



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:20 PM UTC

PDB ID : 9S0V / pdb_00009s0v
Title : The Crystal Structure of Human Tissue Nonspecific Alkaline Phosphatase (hT-NAP) in complex with phosphate
Authors : Ballut, L.; Violot, S.; Imam, I.
Deposited on : 2025-07-17
Resolution : 3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

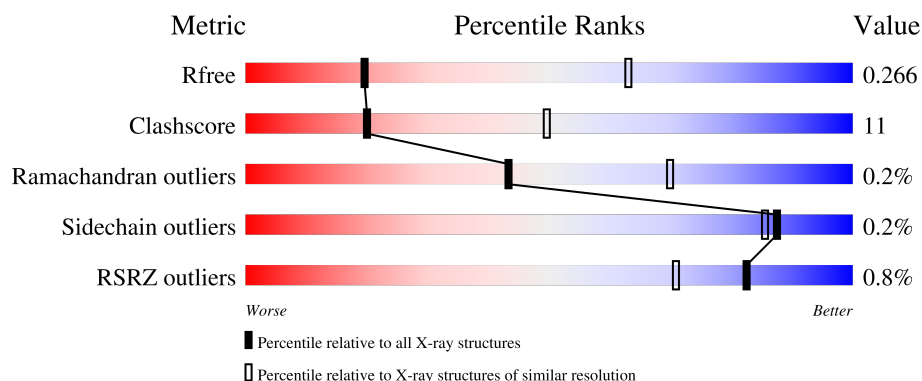
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



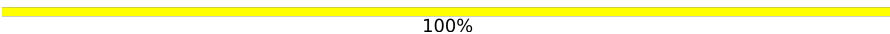
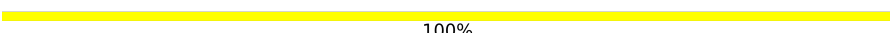
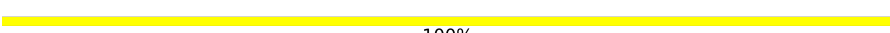
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	509	
1	B	509	
1	C	509	
1	D	509	
1	E	509	

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Mol	Chain	Length	Quality of chain
2	F	2	 50% 50%
2	G	2	 100%
2	I	2	 50% 50%
2	J	2	 100%
2	L	2	 50% 50%
2	M	2	 100%
2	N	2	 100%
2	O	2	 100%
2	P	2	 100%
2	R	2	 50% 50%
3	H	3	 100%
3	K	3	 33% 67%
3	Q	3	 67% 33%
3	S	3	 100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19230 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alkaline phosphatase, tissue-nonspecific isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3709	2320	658	712	19			
1	B	482	Total	C	N	O	S	0	0	0
			3734	2337	663	715	19			
1	C	482	Total	C	N	O	S	0	0	0
			3738	2339	663	717	19			
1	D	483	Total	C	N	O	S	0	0	0
			3737	2339	661	718	19			
1	E	482	Total	C	N	O	S	0	0	0
			3738	2339	663	717	19			

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	ALA	-	expression tag	UNP P05186
A	502	ALA	-	expression tag	UNP P05186
A	503	ALA	-	expression tag	UNP P05186
A	504	GLU	-	expression tag	UNP P05186
A	505	ASN	-	expression tag	UNP P05186
A	506	LEU	-	expression tag	UNP P05186
A	507	TYR	-	expression tag	UNP P05186
A	508	PHE	-	expression tag	UNP P05186
A	509	GLN	-	expression tag	UNP P05186
A	510	GLY	-	expression tag	UNP P05186
A	511	ASP	-	expression tag	UNP P05186
A	512	TYR	-	expression tag	UNP P05186
A	513	LYS	-	expression tag	UNP P05186
A	514	ASP	-	expression tag	UNP P05186
A	515	ASP	-	expression tag	UNP P05186
A	516	ASP	-	expression tag	UNP P05186
A	517	ASP	-	expression tag	UNP P05186
A	518	LYS	-	expression tag	UNP P05186
A	519	HIS	-	expression tag	UNP P05186

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Chain	Residue	Modelled	Actual	Comment	Reference
A	520	HIS	-	expression tag	UNP P05186
A	521	HIS	-	expression tag	UNP P05186
A	522	HIS	-	expression tag	UNP P05186
A	523	HIS	-	expression tag	UNP P05186
A	524	HIS	-	expression tag	UNP P05186
A	525	HIS	-	expression tag	UNP P05186
A	526	HIS	-	expression tag	UNP P05186
B	501	ALA	-	expression tag	UNP P05186
B	502	ALA	-	expression tag	UNP P05186
B	503	ALA	-	expression tag	UNP P05186
B	504	GLU	-	expression tag	UNP P05186
B	505	ASN	-	expression tag	UNP P05186
B	506	LEU	-	expression tag	UNP P05186
B	507	TYR	-	expression tag	UNP P05186
B	508	PHE	-	expression tag	UNP P05186
B	509	GLN	-	expression tag	UNP P05186
B	510	GLY	-	expression tag	UNP P05186
B	511	ASP	-	expression tag	UNP P05186
B	512	TYR	-	expression tag	UNP P05186
B	513	LYS	-	expression tag	UNP P05186
B	514	ASP	-	expression tag	UNP P05186
B	515	ASP	-	expression tag	UNP P05186
B	516	ASP	-	expression tag	UNP P05186
B	517	ASP	-	expression tag	UNP P05186
B	518	LYS	-	expression tag	UNP P05186
B	519	HIS	-	expression tag	UNP P05186
B	520	HIS	-	expression tag	UNP P05186
B	521	HIS	-	expression tag	UNP P05186
B	522	HIS	-	expression tag	UNP P05186
B	523	HIS	-	expression tag	UNP P05186
B	524	HIS	-	expression tag	UNP P05186
B	525	HIS	-	expression tag	UNP P05186
B	526	HIS	-	expression tag	UNP P05186
C	501	ALA	-	expression tag	UNP P05186
C	502	ALA	-	expression tag	UNP P05186
C	503	ALA	-	expression tag	UNP P05186
C	504	GLU	-	expression tag	UNP P05186
C	505	ASN	-	expression tag	UNP P05186
C	506	LEU	-	expression tag	UNP P05186
C	507	TYR	-	expression tag	UNP P05186
C	508	PHE	-	expression tag	UNP P05186
C	509	GLN	-	expression tag	UNP P05186

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Chain	Residue	Modelled	Actual	Comment	Reference
C	510	GLY	-	expression tag	UNP P05186
C	511	ASP	-	expression tag	UNP P05186
C	512	TYR	-	expression tag	UNP P05186
C	513	LYS	-	expression tag	UNP P05186
C	514	ASP	-	expression tag	UNP P05186
C	515	ASP	-	expression tag	UNP P05186
C	516	ASP	-	expression tag	UNP P05186
C	517	ASP	-	expression tag	UNP P05186
C	518	LYS	-	expression tag	UNP P05186
C	519	HIS	-	expression tag	UNP P05186
C	520	HIS	-	expression tag	UNP P05186
C	521	HIS	-	expression tag	UNP P05186
C	522	HIS	-	expression tag	UNP P05186
C	523	HIS	-	expression tag	UNP P05186
C	524	HIS	-	expression tag	UNP P05186
C	525	HIS	-	expression tag	UNP P05186
C	526	HIS	-	expression tag	UNP P05186
D	501	ALA	-	expression tag	UNP P05186
D	502	ALA	-	expression tag	UNP P05186
D	503	ALA	-	expression tag	UNP P05186
D	504	GLU	-	expression tag	UNP P05186
D	505	ASN	-	expression tag	UNP P05186
D	506	LEU	-	expression tag	UNP P05186
D	507	TYR	-	expression tag	UNP P05186
D	508	PHE	-	expression tag	UNP P05186
D	509	GLN	-	expression tag	UNP P05186
D	510	GLY	-	expression tag	UNP P05186
D	511	ASP	-	expression tag	UNP P05186
D	512	TYR	-	expression tag	UNP P05186
D	513	LYS	-	expression tag	UNP P05186
D	514	ASP	-	expression tag	UNP P05186
D	515	ASP	-	expression tag	UNP P05186
D	516	ASP	-	expression tag	UNP P05186
D	517	ASP	-	expression tag	UNP P05186
D	518	LYS	-	expression tag	UNP P05186
D	519	HIS	-	expression tag	UNP P05186
D	520	HIS	-	expression tag	UNP P05186
D	521	HIS	-	expression tag	UNP P05186
D	522	HIS	-	expression tag	UNP P05186
D	523	HIS	-	expression tag	UNP P05186
D	524	HIS	-	expression tag	UNP P05186
D	525	HIS	-	expression tag	UNP P05186

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Chain	Residue	Modelled	Actual	Comment	Reference
D	526	HIS	-	expression tag	UNP P05186
E	501	ALA	-	expression tag	UNP P05186
E	502	ALA	-	expression tag	UNP P05186
E	503	ALA	-	expression tag	UNP P05186
E	504	GLU	-	expression tag	UNP P05186
E	505	ASN	-	expression tag	UNP P05186
E	506	LEU	-	expression tag	UNP P05186
E	507	TYR	-	expression tag	UNP P05186
E	508	PHE	-	expression tag	UNP P05186
E	509	GLN	-	expression tag	UNP P05186
E	510	GLY	-	expression tag	UNP P05186
E	511	ASP	-	expression tag	UNP P05186
E	512	TYR	-	expression tag	UNP P05186
E	513	LYS	-	expression tag	UNP P05186
E	514	ASP	-	expression tag	UNP P05186
E	515	ASP	-	expression tag	UNP P05186
E	516	ASP	-	expression tag	UNP P05186
E	517	ASP	-	expression tag	UNP P05186
E	518	LYS	-	expression tag	UNP P05186
E	519	HIS	-	expression tag	UNP P05186
E	520	HIS	-	expression tag	UNP P05186
E	521	HIS	-	expression tag	UNP P05186
E	522	HIS	-	expression tag	UNP P05186
E	523	HIS	-	expression tag	UNP P05186
E	524	HIS	-	expression tag	UNP P05186
E	525	HIS	-	expression tag	UNP P05186
E	526	HIS	-	expression tag	UNP P05186

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



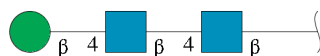
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	S	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Zn	0	0
			2	2		
4	E	2	Total	Zn	0	0
			2	2		

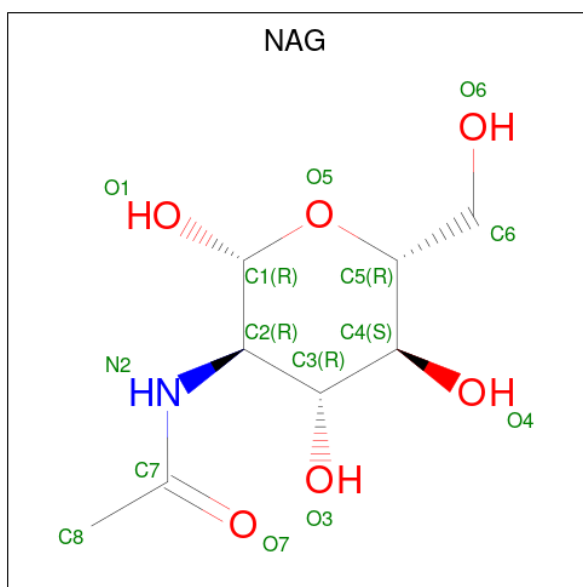
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

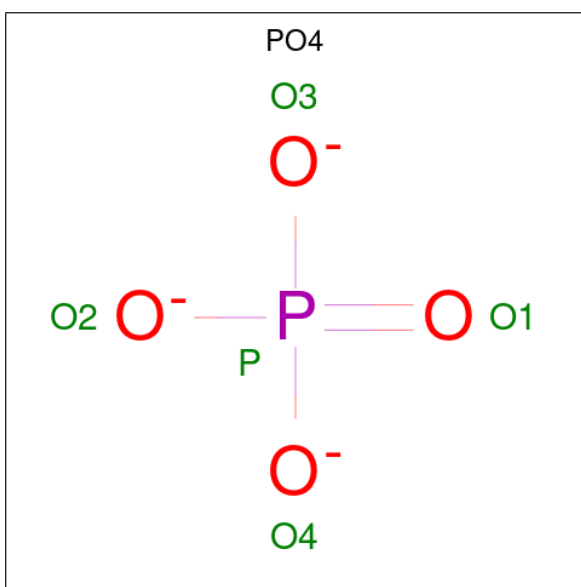
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	P	0	0
			5	4	1		
8	B	1	Total	O	P	0	0
			5	4	1		
8	C	1	Total	O	P	0	0
			5	4	1		
8	D	1	Total	O	P	0	0
			5	4	1		
8	E	1	Total	O	P	0	0
			5	4	1		

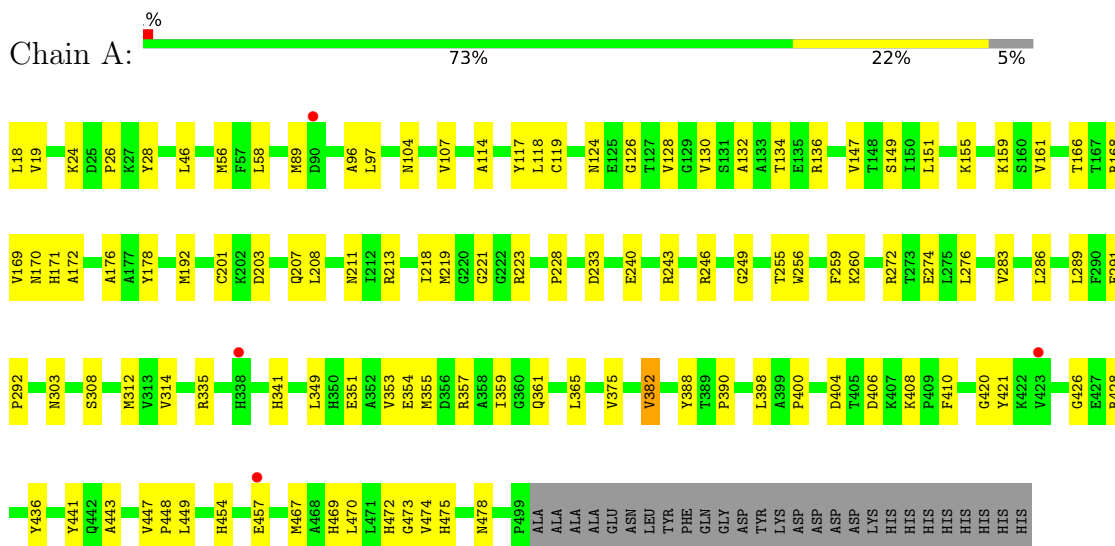
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	O	0	0
			4	4		
9	B	2	Total	O	0	0
			2	2		
9	C	2	Total	O	0	0
			2	2		
9	E	1	Total	O	0	0
			1	1		

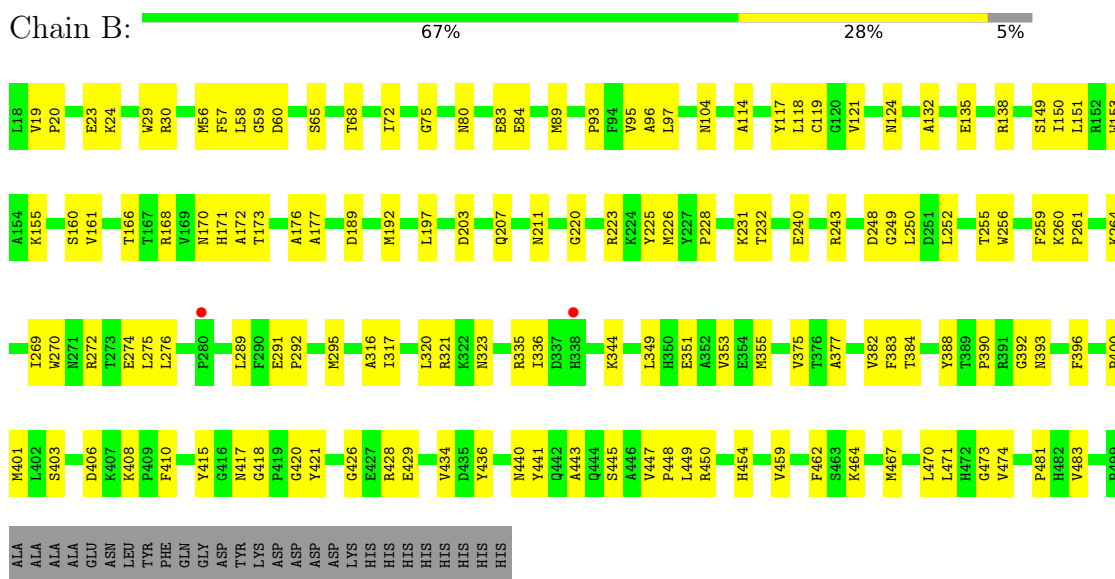
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

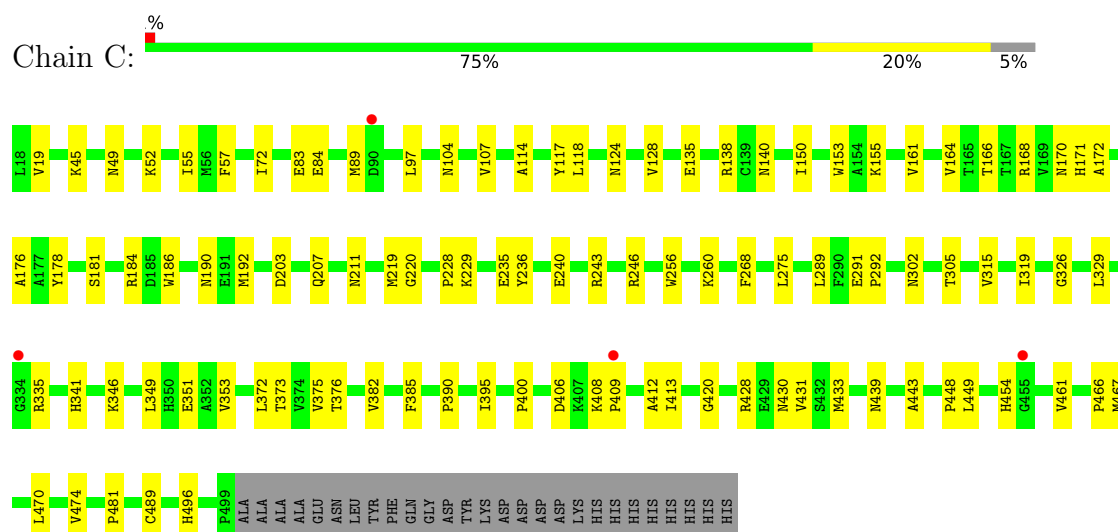
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



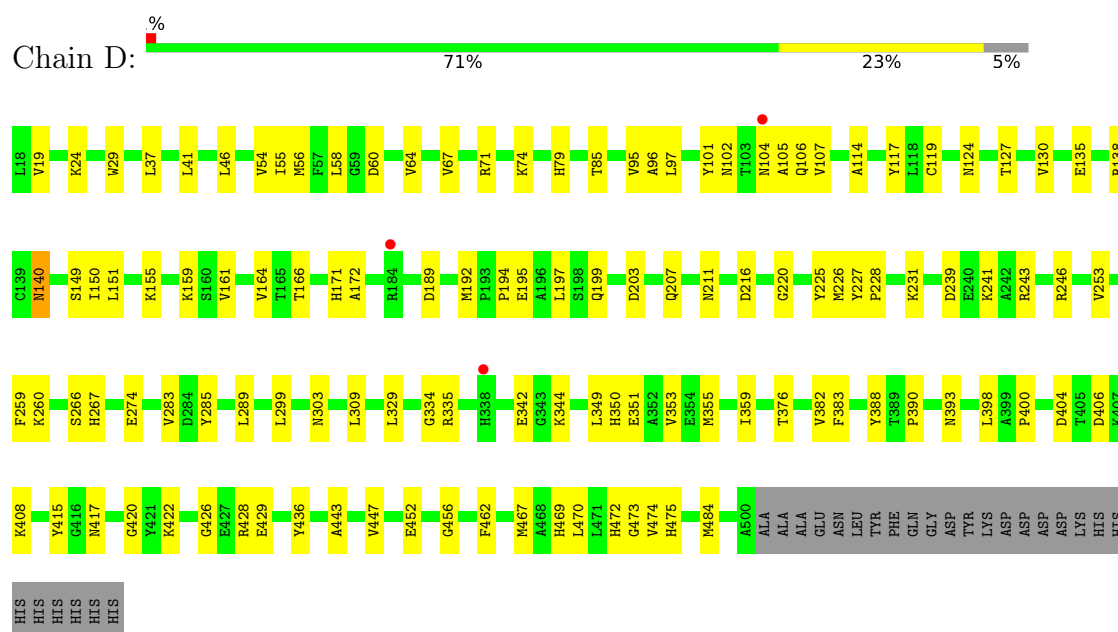
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



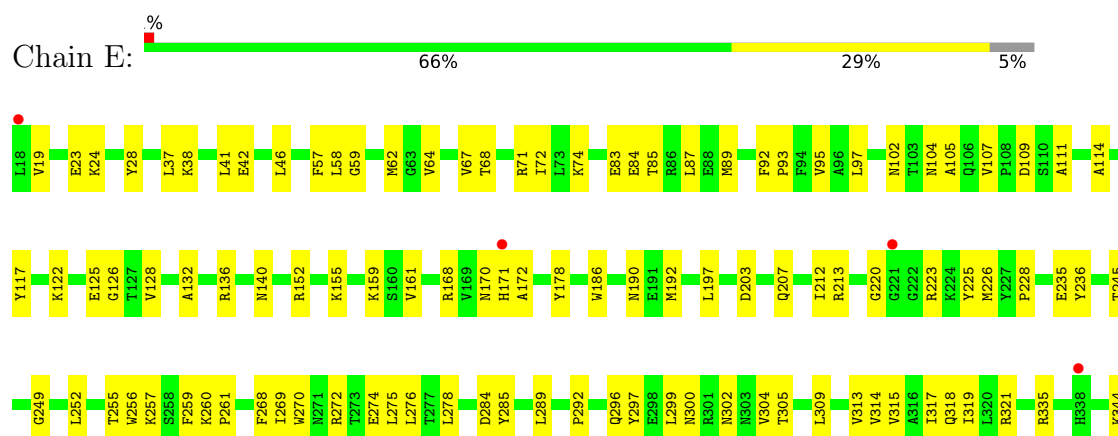
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

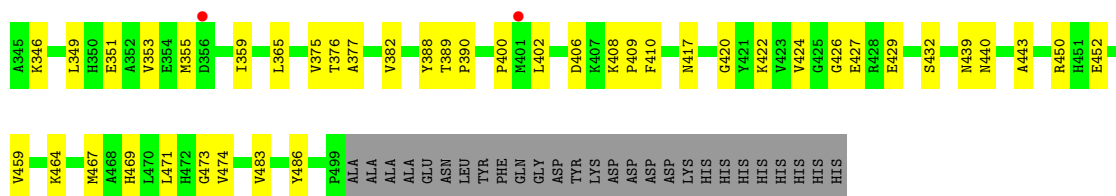


- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



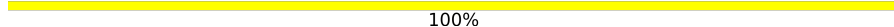


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

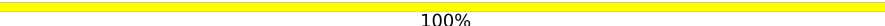
MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

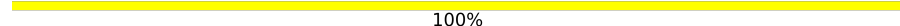
MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

MAG1
MAG2

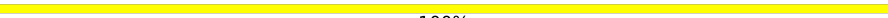
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%MAG1
MAG2

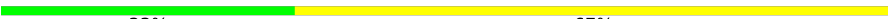
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%MAG1
MAG2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%MAG1
MAG2
BMA3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  33% 67%MAG1
MAG2
BMA3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  67% 33%

MAG1
MAG2
BMA3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	156.73Å 297.70Å 205.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 3.35 39.56 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.56-3.35) 99.6 (39.56-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.215 , 0.266 0.215 , 0.266	Depositor DCC
R_{free} test set	3438 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19230	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BMA, ZN, NAG, CA, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.19	0/3794	0.43	0/5151
1	B	0.20	0/3820	0.44	0/5182
1	C	0.21	0/3824	0.45	0/5187
1	D	0.22	0/3823	0.46	0/5187
1	E	0.21	0/3824	0.46	0/5187
All	All	0.21	0/19085	0.45	0/25894

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3709	0	3570	85	0
1	B	3734	0	3614	110	0
1	C	3738	0	3619	66	0
1	D	3737	0	3613	89	0
1	E	3738	0	3618	117	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	I	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	28	0	25	0	0
2	L	28	0	25	2	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	2	0
2	P	28	0	25	0	0
2	R	28	0	25	1	0
3	H	39	0	34	0	0
3	K	39	0	34	0	0
3	Q	39	0	34	1	0
3	S	39	0	34	0	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
7	E	28	0	26	2	0
8	A	5	0	0	1	0
8	B	5	0	0	0	0
8	C	5	0	0	1	0
8	D	5	0	0	0	0
8	E	5	0	0	0	0
9	A	4	0	0	0	0
9	B	2	0	0	0	0
9	C	2	0	0	0	0
9	E	1	0	0	0	0
All	All	19230	0	18498	431	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 11.

All (431) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:LEU:HD11	1:C:315:VAL:HG21	1.45	0.98
1:B:231:LYS:HG3	1:B:232:THR:H	1.23	0.97
1:A:426:GLY:HA2	1:B:426:GLY:HA2	1.50	0.93
1:E:152:ARG:HD2	1:E:212:ILE:HD11	1.55	0.89
1:B:272:ARG:HE	1:B:276:LEU:HD11	1.37	0.88
1:A:24:LYS:HA	1:B:132:ALA:HB3	1.60	0.84
1:D:19:VAL:CG1	1:D:24:LYS:HE2	2.10	0.80
1:E:102:ASN:HB2	1:E:105:ALA:HB3	1.63	0.80
1:D:104:ASN:OD1	1:E:19:VAL:HG22	1.83	0.78
1:A:426:GLY:CA	1:B:426:GLY:HA2	2.15	0.77
1:D:398:LEU:HD11	1:D:436:TYR:CZ	2.21	0.76
1:C:390:PRO:HD3	1:C:400:PRO:HG3	1.66	0.76
1:D:426:GLY:HA2	1:E:426:GLY:HA2	1.68	0.75
1:A:58:LEU:HD21	1:A:117:TYR:CE1	2.22	0.75
1:B:97:LEU:HB2	1:B:474:VAL:HG22	1.69	0.74
1:B:151:LEU:HD11	1:B:161:VAL:HB	1.67	0.74
1:D:150:ILE:HD13	1:D:484:MET:HE2	1.71	0.73
1:B:421:TYR:CG	1:B:448:PRO:HG3	2.25	0.72
2:O:1:NAG:H61	2:O:2:NAG:O5	1.90	0.72
1:B:114:ALA:HA	1:B:117:TYR:CZ	2.25	0.71
1:E:390:PRO:HD3	1:E:400:PRO:HG3	1.73	0.71
1:E:126:GLY:HA3	1:E:136:ARG:HD2	1.73	0.70
1:C:114:ALA:HA	1:C:117:TYR:CZ	2.27	0.70
1:B:316:ALA:O	1:B:320:LEU:HD12	1.91	0.69
1:B:104:ASN:ND2	1:B:124:ASN:HB3	2.07	0.69
1:C:104:ASN:ND2	1:C:124:ASN:HB3	2.09	0.68
1:B:124:ASN:OD1	1:B:132:ALA:HA	1.93	0.68
1:A:132:ALA:HB3	1:B:24:LYS:HA	1.75	0.68
1:D:19:VAL:HG12	1:D:24:LYS:HE2	1.74	0.68
1:A:255:THR:HG22	1:A:259:PHE:HE2	1.59	0.68
1:A:114:ALA:HA	1:A:117:TYR:CZ	2.29	0.67
1:C:430:ASN:HB3	1:C:433:MET:HE2	1.75	0.67
1:E:58:LEU:HD12	1:E:376:THR:HG23	1.76	0.67
1:E:192:MET:HE2	1:E:203:ASP:HB3	1.77	0.67
1:E:422:LYS:HE2	1:E:424:VAL:HG12	1.76	0.67
1:B:231:LYS:HG3	1:B:232:THR:N	2.01	0.66
1:D:390:PRO:HD3	1:D:400:PRO:HG3	1.77	0.66
1:E:46:LEU:HD13	1:E:469:HIS:CD2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:THR:HG22	1:A:259:PHE:CE2	2.31	0.66
1:A:390:PRO:HD3	1:A:400:PRO:HG3	1.77	0.66
1:B:406:ASP:OD2	1:B:428:ARG:HD3	1.96	0.66
1:E:260:LYS:HD2	1:E:285:TYR:CD2	2.31	0.66
1:D:41:LEU:HD21	1:E:486:TYR:HE2	1.61	0.66
1:C:406:ASP:OD2	1:C:428:ARG:HD3	1.97	0.64
1:D:231:LYS:O	1:D:243:ARG:HA	1.97	0.64
1:B:57:PHE:HB3	1:B:355:MET:HE2	1.80	0.64
1:D:114:ALA:HA	1:D:117:TYR:CZ	2.33	0.64
1:D:19:VAL:HG11	1:D:24:LYS:HE2	1.82	0.62
1:D:189:ASP:HA	1:D:192:MET:HE2	1.80	0.62
1:E:255:THR:O	1:E:259:PHE:HD1	1.81	0.62
7:E:605:NAG:C1	7:E:605:NAG:O7	2.47	0.62
1:B:261:PRO:HG2	1:B:264:LYS:HB2	1.81	0.61
4:A:601:ZN:ZN	8:A:606:PO4:O1	1.49	0.61
1:A:274:GLU:OE2	2:F:1:NAG:H61	2.00	0.61
1:E:59:GLY:HA3	1:E:62:MET:HE3	1.81	0.61
1:E:318:GLN:HA	1:E:321:ARG:HH11	1.65	0.61
1:B:117:TYR:HA	1:B:481:PRO:HD3	1.84	0.60
1:E:299:LEU:HD13	1:E:439:ASN:HD22	1.68	0.59
1:B:171:HIS:CG	1:B:172:ALA:H	2.21	0.59
1:B:276:LEU:O	1:C:45:LYS:HE3	2.02	0.59
1:D:274:GLU:OE2	2:O:1:NAG:H62	2.02	0.59
1:B:256:TRP:CD1	1:B:260:LYS:HZ1	2.20	0.59
1:C:104:ASN:HD21	1:C:124:ASN:HB3	1.67	0.59
1:E:269:ILE:HD12	1:E:275:LEU:HB2	1.85	0.59
1:A:406:ASP:OD2	1:A:428:ARG:HD3	2.03	0.59
1:E:114:ALA:HA	1:E:117:TYR:CZ	2.37	0.59
1:C:140:ASN:HD21	2:L:1:NAG:C6	2.15	0.59
1:E:226:MET:HA	1:E:252:LEU:HD12	1.86	0.58
1:E:272:ARG:NH1	1:E:276:LEU:HD11	2.18	0.58
1:A:97:LEU:HD12	1:B:95:VAL:HG11	1.85	0.58
1:D:135:GLU:HB2	1:D:138:ARG:HG3	1.86	0.58
1:D:71:ARG:HD3	1:D:85:THR:O	2.04	0.58
1:E:296:GLN:HB3	1:E:300:ASN:HB2	1.84	0.57
1:C:315:VAL:O	1:C:319:ILE:HG13	2.04	0.57
1:E:255:THR:HG22	1:E:259:PHE:HE1	1.70	0.57
1:C:268:PHE:HE1	1:C:289:LEU:HD12	1.69	0.57
1:B:226:MET:HA	1:B:252:LEU:HD12	1.87	0.56
1:E:89:MET:HE2	1:E:375:VAL:HG11	1.86	0.56
1:A:208:LEU:HD11	1:A:218:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PRO:HB3	1:A:249:GLY:HA2	1.88	0.56
1:E:46:LEU:HD13	1:E:469:HIS:HD2	1.70	0.56
1:B:155:LYS:HD3	1:B:161:VAL:HG22	1.88	0.56
1:E:155:LYS:HD3	1:E:161:VAL:HG22	1.86	0.56
1:A:124:ASN:OD1	1:A:132:ALA:HA	2.06	0.55
1:D:64:VAL:HA	1:D:67:VAL:HG22	1.89	0.55
1:B:56:MET:HE1	1:B:117:TYR:CD1	2.41	0.55
1:E:344:LYS:HD3	1:E:440:ASN:HA	1.89	0.55
1:A:89:MET:HE2	1:A:375:VAL:HG11	1.88	0.55
1:A:104:ASN:ND2	1:A:124:ASN:HB3	2.22	0.55
1:E:349:LEU:O	1:E:353:VAL:HG23	2.07	0.55
1:C:240:GLU:HA	1:C:243:ARG:HG3	1.89	0.55
1:B:383:PHE:HB2	1:B:415:TYR:CE1	2.42	0.54
1:A:256:TRP:CD1	1:A:260:LYS:HZ3	2.25	0.54
1:C:346:LYS:HD3	1:C:439:ASN:HA	1.89	0.54
1:E:152:ARG:CD	1:E:212:ILE:HD11	2.35	0.54
1:E:223:ARG:HB2	1:E:292:PRO:HA	1.90	0.54
1:E:313:VAL:O	1:E:317:ILE:HG13	2.07	0.54
1:B:68:THR:O	1:B:72:ILE:HG12	2.08	0.54
1:C:256:TRP:CD1	1:C:260:LYS:HZ3	2.26	0.54
1:A:467:MET:HE3	1:A:470:LEU:HD11	1.90	0.54
1:E:408:LYS:NZ	1:E:427:GLU:HB3	2.22	0.54
1:B:291:GLU:HG3	1:B:295:MET:HA	1.90	0.54
1:E:213:ARG:HD2	1:E:259:PHE:CD2	2.43	0.54
1:A:119:CYS:HA	1:A:149:SER:HA	1.90	0.54
1:A:314:VAL:HG13	1:A:365:LEU:HD11	1.90	0.54
1:B:89:MET:HE2	1:B:375:VAL:HG11	1.89	0.54
1:D:195:GLU:O	1:D:199:GLN:HG2	2.08	0.54
1:E:467:MET:HA	1:E:469:HIS:CE1	2.41	0.54
1:D:406:ASP:OD2	1:D:428:ARG:HD3	2.07	0.53
1:A:420:GLY:HA3	1:A:443:ALA:O	2.09	0.53
1:A:147:VAL:HG13	1:B:30:ARG:HH21	1.74	0.53
1:A:291:GLU:HG3	1:A:292:PRO:HD2	1.90	0.53
1:D:390:PRO:HG2	1:D:393:ASN:HB2	1.91	0.53
1:B:417:ASN:HB2	1:B:449:LEU:CD1	2.38	0.53
1:E:190:ASN:HB2	1:E:245:THR:O	2.08	0.53
1:B:269:ILE:HD12	1:B:275:LEU:HB2	1.89	0.53
1:D:101:TYR:CD2	1:E:83:GLU:HB3	2.43	0.53
1:C:140:ASN:HD21	2:L:1:NAG:H61	1.74	0.53
1:E:171:HIS:CG	1:E:172:ALA:H	2.27	0.53
1:D:119:CYS:HA	1:D:149:SER:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:HG21	1:B:410:PHE:HB2	1.91	0.53
1:C:168:ARG:HB3	1:C:170:ASN:OD1	2.09	0.52
1:A:410:PHE:HB2	1:B:447:VAL:HG21	1.92	0.52
1:D:422:LYS:HG2	1:D:429:GLU:OE1	2.09	0.52
1:D:19:VAL:HG12	1:D:24:LYS:CE	2.39	0.52
1:B:166:THR:OG1	1:B:335:ARG:HG2	2.09	0.52
1:A:474:VAL:HG23	1:B:95:VAL:HG21	1.92	0.52
1:A:404:ASP:HB2	1:B:450:ARG:HG3	1.92	0.52
1:B:467:MET:HE3	1:B:470:LEU:HD11	1.92	0.52
1:C:84:GLU:CD	1:C:84:GLU:H	2.17	0.52
1:A:126:GLY:HA3	1:A:136:ARG:HD2	1.91	0.52
1:D:383:PHE:HB2	1:D:415:TYR:CE1	2.44	0.52
1:E:23:GLU:HG2	1:E:28:TYR:CE2	2.46	0.52
1:E:406:ASP:HB2	1:E:408:LYS:HE3	1.92	0.52
1:B:203:ASP:O	1:B:207:GLN:HG3	2.10	0.51
1:B:84:GLU:CD	1:B:84:GLU:H	2.19	0.51
1:C:302:ASN:HB3	1:C:305:THR:OG1	2.10	0.51
1:E:235:GLU:HG2	1:E:236:TYR:CE1	2.46	0.51
1:E:257:LYS:HA	1:E:260:LYS:HG2	1.93	0.51
1:A:114:ALA:HA	1:A:117:TYR:CE1	2.45	0.51
1:C:155:LYS:HD3	1:C:161:VAL:HG22	1.93	0.51
1:B:57:PHE:HB3	1:B:355:MET:CE	2.41	0.51
1:B:255:THR:HG22	1:B:259:PHE:CE2	2.45	0.51
1:D:267:HIS:CE1	1:D:283:VAL:HG22	2.46	0.51
1:B:441:TYR:HE1	1:B:443:ALA:HA	1.76	0.51
1:E:64:VAL:HA	1:E:67:VAL:HG22	1.91	0.51
1:E:315:VAL:O	1:E:319:ILE:HG13	2.11	0.51
1:B:421:TYR:CD1	1:B:448:PRO:HG3	2.46	0.51
1:E:299:LEU:HD13	1:E:439:ASN:ND2	2.26	0.51
1:A:382:VAL:HG13	1:B:384:THR:OG1	2.11	0.50
1:B:114:ALA:HA	1:B:117:TYR:CE1	2.46	0.50
1:B:135:GLU:HB2	1:B:138:ARG:HG3	1.92	0.50
1:C:395:ILE:HG13	1:C:413:ILE:HD11	1.93	0.50
1:E:471:LEU:CD2	1:E:483:VAL:HG21	2.42	0.50
1:A:28:TYR:HA	1:D:79:HIS:CE1	2.46	0.50
1:E:255:THR:CG2	1:E:259:PHE:HE1	2.24	0.50
1:B:390:PRO:HD3	1:B:400:PRO:HG3	1.92	0.50
1:E:57:PHE:HB3	1:E:355:MET:HE3	1.92	0.50
1:A:207:GLN:HB3	1:A:211:ASN:ND2	2.25	0.50
1:A:228:PRO:HA	1:A:246:ARG:HB2	1.93	0.50
1:B:189:ASP:HA	1:B:192:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:GLU:HA	1:B:243:ARG:HE	1.75	0.50
1:E:417:ASN:O	1:E:452:GLU:HA	2.12	0.50
1:B:104:ASN:HD21	1:B:124:ASN:HB3	1.75	0.50
1:E:97:LEU:HB2	1:E:474:VAL:HG22	1.94	0.50
1:E:422:LYS:HG2	1:E:429:GLU:OE1	2.11	0.50
1:D:225:TYR:HB2	1:D:226:MET:HE2	1.93	0.50
1:E:268:PHE:HE1	1:E:270:TRP:HB3	1.77	0.49
1:C:228:PRO:HA	1:C:246:ARG:HB2	1.94	0.49
1:D:97:LEU:HB2	1:D:474:VAL:HG22	1.93	0.49
1:A:272:ARG:CZ	1:A:276:LEU:HD11	2.42	0.49
1:D:140:ASN:OD1	1:D:140:ASN:N	2.44	0.49
1:D:29:TRP:CZ3	1:E:122:LYS:HG3	2.47	0.49
1:D:151:LEU:HD11	1:D:161:VAL:HB	1.94	0.49
1:A:192:MET:HE1	1:A:201:CYS:O	2.12	0.49
1:C:166:THR:OG1	1:C:335:ARG:HG2	2.12	0.49
1:B:344:LYS:HD3	1:B:440:ASN:HA	1.94	0.49
1:C:184:ARG:NH1	8:C:606:PO4:O3	2.45	0.49
1:D:467:MET:HE3	1:D:470:LEU:HD11	1.95	0.49
1:A:97:LEU:HB2	1:A:474:VAL:HG22	1.94	0.49
1:B:335:ARG:HB2	1:B:351:GLU:OE1	2.13	0.49
1:E:93:PRO:HD2	1:E:464:LYS:HB3	1.94	0.49
1:E:220:GLY:O	1:E:289:LEU:HA	2.12	0.49
1:E:469:HIS:H	1:E:469:HIS:HD1	1.59	0.49
1:D:355:MET:HE3	1:D:359:ILE:HD11	1.95	0.49
1:A:308:SER:HB2	1:A:354:GLU:OE2	2.13	0.49
1:E:23:GLU:HG2	1:E:28:TYR:HE2	1.77	0.49
1:E:57:PHE:HB3	1:E:355:MET:CE	2.42	0.49
1:B:406:ASP:HB2	1:B:408:LYS:HE2	1.94	0.48
1:C:256:TRP:O	1:C:260:LYS:HG2	2.13	0.48
1:A:223:ARG:HD2	1:A:233:ASP:OD1	2.13	0.48
1:D:260:LYS:HD2	1:D:285:TYR:CD2	2.48	0.48
1:A:118:LEU:HD12	1:A:176:ALA:HB3	1.94	0.48
1:E:377:ALA:O	1:E:459:VAL:HG21	2.14	0.48
1:E:409:PRO:HG3	1:E:432:SER:HB3	1.94	0.48
1:D:417:ASN:O	1:D:452:GLU:HA	2.12	0.48
1:A:46:LEU:HB3	1:A:469:HIS:CE1	2.47	0.48
1:C:203:ASP:O	1:C:207:GLN:HG3	2.13	0.48
1:A:349:LEU:O	1:A:353:VAL:HG23	2.13	0.48
1:A:130:VAL:HG21	1:A:134:THR:HG21	1.96	0.48
1:A:478:ASN:HD22	1:B:29:TRP:HB3	1.79	0.48
1:B:317:ILE:O	1:B:321:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:LEU:HD11	1:D:436:TYR:CE2	2.49	0.48
1:D:420:GLY:HA3	1:D:443:ALA:O	2.13	0.48
1:D:164:VAL:HG23	1:D:329:LEU:HD11	1.95	0.47
1:D:259:PHE:CD1	1:D:259:PHE:N	2.82	0.47
1:D:127:THR:HB	1:D:130:VAL:CG2	2.44	0.47
1:E:171:HIS:CG	1:E:172:ALA:N	2.83	0.47
1:A:436:TYR:HA	1:A:441:TYR:CG	2.49	0.47
1:E:346:LYS:HD3	1:E:439:ASN:HA	1.96	0.47
1:C:406:ASP:HB2	1:C:408:LYS:HE2	1.97	0.47
1:D:95:VAL:HG22	1:D:462:PHE:HD1	1.79	0.47
1:E:261:PRO:HD2	1:E:285:TYR:HE2	1.80	0.47
1:D:56:MET:HE3	1:D:484:MET:HE1	1.96	0.47
1:D:227:TYR:CZ	1:D:253:VAL:HG21	2.49	0.47
1:D:266:SER:HB3	1:D:285:TYR:HB2	1.97	0.47
1:D:447:VAL:HG21	1:E:410:PHE:HB2	1.95	0.47
1:D:106:GLN:HB3	1:E:389:THR:OG1	2.14	0.47
1:D:171:HIS:CG	1:D:172:ALA:H	2.33	0.47
1:E:256:TRP:O	1:E:260:LYS:HE2	2.15	0.47
1:B:220:GLY:O	1:B:289:LEU:HA	2.15	0.47
1:B:415:TYR:O	1:B:445:SER:HA	2.15	0.47
1:B:228:PRO:HB3	1:B:249:GLY:HA2	1.96	0.47
1:C:467:MET:HE3	1:C:470:LEU:HD11	1.97	0.47
1:D:102:ASN:HB2	1:D:105:ALA:HB3	1.97	0.47
1:D:166:THR:OG1	1:D:335:ARG:HG2	2.14	0.47
1:E:471:LEU:HD21	1:E:483:VAL:HG21	1.96	0.47
1:A:219:MET:SD	1:A:312:MET:HG2	2.55	0.46
1:A:449:LEU:HD23	1:B:403:SER:HB2	1.97	0.46
1:C:341:HIS:HE1	1:C:454:HIS:CD2	2.33	0.46
1:A:28:TYR:HA	1:D:79:HIS:ND1	2.29	0.46
1:A:147:VAL:HG13	1:B:30:ARG:NH2	2.29	0.46
1:A:406:ASP:HB2	1:A:408:LYS:HE2	1.97	0.46
1:E:335:ARG:HB2	1:E:351:GLU:CD	2.39	0.46
1:A:128:VAL:HG13	1:A:176:ALA:HA	1.97	0.46
1:B:119:CYS:HA	1:B:149:SER:HA	1.97	0.46
1:D:216:ASP:HA	1:D:285:TYR:CD1	2.50	0.46
1:A:169:VAL:HG13	1:A:221:GLY:O	2.15	0.46
1:B:349:LEU:HD12	1:B:396:PHE:CE1	2.51	0.46
1:D:104:ASN:ND2	1:D:124:ASN:HB3	2.30	0.46
1:B:436:TYR:HA	1:B:441:TYR:CD2	2.50	0.46
1:E:255:THR:O	1:E:259:PHE:CD1	2.67	0.46
1:A:151:LEU:HD11	1:A:161:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:GLU:HG2	1:B:65:SER:HA	1.97	0.46
1:B:256:TRP:O	1:B:260:LYS:HG2	2.15	0.46
1:C:186:TRP:CG	1:C:192:MET:HG2	2.51	0.46
1:C:376:THR:OG1	1:C:461:VAL:HG22	2.16	0.46
1:D:239:ASP:OD1	1:D:241:LYS:HE2	2.16	0.46
1:A:398:LEU:HD11	1:A:436:TYR:CE2	2.51	0.46
1:B:59:GLY:N	1:B:355:MET:HE1	2.30	0.46
1:B:274:GLU:OE2	2:I:1:NAG:H62	2.16	0.46
1:A:96:ALA:HB1	1:A:473:GLY:O	2.15	0.46
1:B:248:ASP:OD2	1:B:250:LEU:HD12	2.16	0.46
1:D:37:LEU:HD21	1:E:483:VAL:HG22	1.97	0.46
1:D:194:PRO:HA	1:D:197:LEU:HD21	1.98	0.46
1:E:270:TRP:HE1	2:R:1:NAG:H61	1.81	0.46
1:C:117:TYR:HA	1:C:481:PRO:HD3	1.98	0.45
1:D:228:PRO:HA	1:D:246:ARG:HB2	1.97	0.45
1:D:473:GLY:HA2	1:E:95:VAL:HG23	1.98	0.45
1:C:89:MET:HE2	1:C:375:VAL:HG11	1.98	0.45
1:D:107:VAL:HB	1:E:388:TYR:HA	1.98	0.45
1:A:255:THR:O	1:A:259:PHE:CD2	2.69	0.45
1:D:203:ASP:O	1:D:207:GLN:HG3	2.15	0.45
1:A:26:PRO:HB3	1:B:121:VAL:HG21	1.99	0.45
1:B:160:SER:OG	1:B:323:ASN:HB2	2.17	0.45
1:C:220:GLY:O	1:C:289:LEU:HA	2.15	0.45
1:C:335:ARG:HB2	1:C:351:GLU:OE1	2.16	0.45
1:D:388:TYR:HA	1:E:107:VAL:HB	1.97	0.45
1:A:168:ARG:HB3	1:A:170:ASN:OD1	2.16	0.45
1:D:349:LEU:O	1:D:353:VAL:HG23	2.17	0.45
1:E:192:MET:HE3	1:E:197:LEU:HD21	1.97	0.45
1:A:472:HIS:HE1	1:A:475:HIS:HE1	1.65	0.45
1:B:225:TYR:HB2	1:B:226:MET:HE2	1.99	0.45
1:B:60:ASP:O	1:B:336:ILE:HB	2.17	0.45
1:B:72:ILE:HD12	1:B:83:GLU:HG3	1.99	0.45
1:D:342:GLU:HB3	1:D:344:LYS:HE3	1.98	0.45
1:A:355:MET:O	1:A:359:ILE:HG13	2.17	0.45
1:C:135:GLU:HB2	1:C:138:ARG:CD	2.47	0.45
1:C:118:LEU:HD12	1:C:176:ALA:HB3	1.99	0.45
1:D:95:VAL:HG23	1:E:473:GLY:HA2	1.99	0.45
1:D:299:LEU:HD21	1:D:350:HIS:CD2	2.52	0.45
1:A:166:THR:OG1	1:A:335:ARG:HG2	2.18	0.44
1:C:448:PRO:O	1:C:449:LEU:HD23	2.17	0.44
1:E:38:LYS:O	1:E:42:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:GLU:CD	1:E:84:GLU:H	2.25	0.44
1:E:186:TRP:CG	1:E:192:MET:HG2	2.52	0.44
1:A:421:TYR:CD2	1:A:448:PRO:HB3	2.53	0.44
1:B:20:PRO:HB2	1:B:23:GLU:HG3	1.98	0.44
1:A:104:ASN:OD1	1:B:19:VAL:HG22	2.17	0.44
1:E:93:PRO:HD2	1:E:464:LYS:CB	2.48	0.44
1:E:168:ARG:HD2	1:E:225:TYR:HE2	1.83	0.44
1:E:256:TRP:O	1:E:260:LYS:HG2	2.17	0.44
1:B:349:LEU:O	1:B:353:VAL:HG23	2.17	0.44
1:D:54:VAL:HG11	1:D:484:MET:HE3	1.98	0.44
1:B:72:ILE:HD13	1:B:83:GLU:HA	1.99	0.44
1:C:150:ILE:HA	1:C:153:TRP:CE3	2.53	0.44
1:E:74:LYS:HD2	1:E:87:LEU:HD23	1.99	0.44
1:B:255:THR:HG22	1:B:259:PHE:HE2	1.81	0.44
1:C:170:ASN:HA	1:C:178:TYR:OH	2.18	0.44
1:D:95:VAL:HG21	1:E:474:VAL:HG23	1.99	0.44
1:E:203:ASP:O	1:E:207:GLN:HG3	2.18	0.44
1:A:119:CYS:HB3	1:A:147:VAL:HG12	2.00	0.44
1:A:155:LYS:HD2	1:A:159:LYS:O	2.17	0.44
1:C:291:GLU:HG3	1:C:292:PRO:HD2	1.99	0.44
1:E:37:LEU:O	1:E:41:LEU:HD12	2.18	0.44
1:E:104:ASN:HD21	1:E:125:GLU:HG2	1.82	0.44
1:D:266:SER:HA	1:D:285:TYR:O	2.18	0.44
1:D:408:LYS:CG	3:Q:1:NAG:H82	2.48	0.44
1:B:171:HIS:CG	1:B:172:ALA:N	2.82	0.43
1:D:106:GLN:NE2	1:E:72:ILE:HD13	2.33	0.43
1:E:355:MET:O	1:E:359:ILE:HG13	2.18	0.43
1:B:96:ALA:HB1	1:B:473:GLY:O	2.18	0.43
1:C:55:ILE:HB	1:C:373:THR:HG23	2.00	0.43
1:C:409:PRO:HG2	1:C:431:VAL:HG23	2.00	0.43
1:D:155:LYS:HD2	1:D:159:LYS:O	2.18	0.43
1:E:297:TYR:CE1	1:E:335:ARG:HB3	2.53	0.43
1:E:314:VAL:HG13	1:E:365:LEU:HD11	2.00	0.43
1:A:213:ARG:HD3	1:A:259:PHE:CD1	2.53	0.43
1:A:388:TYR:HE1	1:B:454:HIS:H	1.64	0.43
1:C:150:ILE:HA	1:C:153:TRP:CD2	2.53	0.43
1:C:164:VAL:HG23	1:C:329:LEU:HD11	2.00	0.43
1:D:96:ALA:HB1	1:D:473:GLY:O	2.18	0.43
1:E:111:ALA:HB1	1:E:128:VAL:CG2	2.48	0.43
1:B:223:ARG:NH1	1:B:270:TRP:HB2	2.33	0.43
1:C:155:LYS:HD2	1:C:155:LYS:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:GLU:HG2	1:C:236:TYR:CE1	2.54	0.43
1:E:140:ASN:ND2	7:E:605:NAG:H61	2.34	0.43
1:E:297:TYR:HB2	1:E:300:ASN:ND2	2.33	0.43
1:E:302:ASN:HB3	1:E:305:THR:OG1	2.18	0.43
1:A:357:ARG:O	1:A:361:GLN:HG3	2.18	0.43
1:B:418:GLY:H	1:B:445:SER:HB2	1.84	0.43
1:C:335:ARG:HB2	1:C:351:GLU:CD	2.44	0.43
1:D:456:GLY:O	1:E:68:THR:HG21	2.18	0.43
1:D:472:HIS:O	1:D:475:HIS:CD2	2.72	0.43
1:E:228:PRO:HB3	1:E:249:GLY:HA2	1.99	0.43
1:A:240:GLU:HA	1:A:243:ARG:HD2	2.00	0.43
1:B:118:LEU:HD12	1:B:176:ALA:HB3	2.00	0.43
1:A:335:ARG:HB2	1:A:351:GLU:CD	2.44	0.43
1:B:151:LEU:HD12	1:B:151:LEU:HA	1.76	0.43
1:B:93:PRO:HD2	1:B:464:LYS:HB3	2.01	0.43
1:B:377:ALA:O	1:B:459:VAL:HG21	2.19	0.43
1:D:383:PHE:HB2	1:D:415:TYR:HE1	1.82	0.43
1:A:56:MET:HG2	1:A:58:LEU:CD1	2.48	0.43
1:B:207:GLN:HB3	1:B:211:ASN:ND2	2.34	0.43
1:C:171:HIS:CG	1:C:172:ALA:H	2.37	0.43
1:C:268:PHE:CE1	1:C:289:LEU:HD12	2.52	0.43
1:A:283:VAL:HG11	1:A:286:LEU:HB2	2.01	0.42
1:B:57:PHE:HB2	1:B:375:VAL:HG22	2.00	0.42
1:B:168:ARG:HB3	1:B:170:ASN:OD1	2.19	0.42
1:D:335:ARG:HB2	1:D:351:GLU:OE1	2.18	0.42
1:A:18:LEU:HB3	1:A:19:VAL:H	1.72	0.42
1:C:420:GLY:HA3	1:C:443:ALA:O	2.19	0.42
1:D:207:GLN:HB3	1:D:211:ASN:ND2	2.34	0.42
1:E:309:LEU:O	1:E:313:VAL:HG23	2.19	0.42
1:A:58:LEU:CD2	1:A:117:TYR:CE1	3.00	0.42
1:B:150:ILE:HA	1:B:153:TRP:CD2	2.53	0.42
1:C:19:VAL:HG23	1:C:19:VAL:O	2.19	0.42
1:E:111:ALA:HB1	1:E:128:VAL:HG23	2.01	0.42
1:E:170:ASN:HA	1:E:178:TYR:OH	2.20	0.42
1:A:349:LEU:HD23	1:A:349:LEU:HA	1.93	0.42
1:D:259:PHE:N	1:D:259:PHE:HD1	2.17	0.42
1:D:404:ASP:HB2	1:E:450:ARG:NH2	2.35	0.42
1:E:424:VAL:HG23	1:E:424:VAL:O	2.19	0.42
1:E:155:LYS:HA	1:E:155:LYS:HD2	1.86	0.42
1:A:472:HIS:CE1	1:A:475:HIS:HE1	2.37	0.42
1:B:401:MET:HE2	1:B:401:MET:HB3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:MET:HE3	1:E:197:LEU:CD2	2.50	0.42
1:B:223:ARG:HB2	1:B:292:PRO:HA	2.01	0.42
1:B:392:GLY:O	1:B:393:ASN:C	2.63	0.42
1:B:441:TYR:CE1	1:B:443:ALA:HA	2.55	0.42
1:C:128:VAL:HG13	1:C:181:SER:H	1.85	0.42
1:C:207:GLN:HB3	1:C:211:ASN:ND2	2.34	0.42
1:E:71:ARG:HD3	1:E:85:THR:O	2.20	0.42
1:E:155:LYS:HD2	1:E:159:LYS:O	2.19	0.42
1:A:46:LEU:HD13	1:A:469:HIS:CD2	2.55	0.42
1:A:178:TYR:CE2	1:A:208:LEU:HD13	2.55	0.42
1:C:349:LEU:O	1:C:353:VAL:HG23	2.20	0.42
1:A:203:ASP:O	1:A:207:GLN:HG3	2.20	0.42
1:D:95:VAL:HG22	1:D:462:PHE:CD1	2.54	0.42
1:A:341:HIS:HE1	1:A:454:HIS:CD2	2.38	0.41
1:C:219:MET:HE1	1:C:315:VAL:HG23	2.02	0.41
1:E:223:ARG:HG2	1:E:289:LEU:HB2	2.01	0.41
1:C:489:CYS:SG	1:C:496:HIS:HB3	2.60	0.41
1:E:304:VAL:HG23	1:E:305:THR:HG23	2.01	0.41
1:A:107:VAL:HB	1:B:388:TYR:HA	2.03	0.41
1:B:275:LEU:HD23	1:B:276:LEU:HD23	2.02	0.41
1:C:219:MET:HE1	1:C:315:VAL:CG2	2.50	0.41
1:B:420:GLY:HA3	1:B:443:ALA:O	2.20	0.41
1:C:107:VAL:HG12	1:C:454:HIS:HB2	2.01	0.41
1:E:420:GLY:HA3	1:E:443:ALA:O	2.20	0.41
1:B:150:ILE:HA	1:B:153:TRP:CE3	2.56	0.41
1:C:97:LEU:HB2	1:C:474:VAL:HG22	2.03	0.41
1:D:46:LEU:HB3	1:D:469:HIS:CE1	2.55	0.41
1:E:19:VAL:HG12	1:E:24:LYS:HE2	2.03	0.41
1:B:95:VAL:HG22	1:B:462:PHE:CD1	2.56	0.41
1:C:49:ASN:O	1:C:466:PRO:HB3	2.21	0.41
1:C:52:LYS:O	1:C:326:GLY:HA3	2.21	0.41
1:C:372:LEU:HB2	1:C:466:PRO:HD2	2.02	0.41
1:C:385:PHE:HA	1:C:412:ALA:O	2.21	0.41
1:D:24:LYS:HA	1:E:132:ALA:HB3	2.03	0.41
1:D:55:ILE:HG12	1:D:329:LEU:HB3	2.03	0.41
1:D:166:THR:HG23	1:D:309:LEU:HD13	2.02	0.41
1:E:402:LEU:H	1:E:402:LEU:HD12	1.86	0.41
1:B:19:VAL:CG1	1:B:24:LYS:HE2	2.50	0.41
1:E:59:GLY:N	1:E:355:MET:HE1	2.35	0.41
1:E:274:GLU:O	1:E:278:LEU:HG	2.21	0.41
1:B:151:LEU:HD22	1:B:177:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:LEU:HD12	1:D:376:THR:HG23	2.03	0.41
1:D:101:TYR:CD1	1:D:101:TYR:C	2.99	0.41
1:D:422:LYS:HE2	1:D:422:LYS:HB2	1.87	0.41
1:E:268:PHE:CD1	1:E:268:PHE:C	2.99	0.41
1:B:58:LEU:HD22	1:B:173:THR:HG21	2.03	0.41
1:B:75:GLY:O	1:B:80:ASN:HB2	2.21	0.41
1:B:117:TYR:CD1	1:B:118:LEU:HG	2.56	0.41
1:B:192:MET:HE3	1:B:197:LEU:CD2	2.50	0.41
1:B:471:LEU:HG	1:B:483:VAL:HG11	2.03	0.41
1:C:57:PHE:HB2	1:C:375:VAL:HG22	2.03	0.41
1:C:72:ILE:CD1	1:C:83:GLU:HG3	2.51	0.41
1:D:74:LYS:HG2	1:D:85:THR:HG21	2.02	0.41
1:E:89:MET:HA	1:E:92:PHE:CD1	2.56	0.41
1:E:284:ASP:O	1:E:285:TYR:CD1	2.73	0.41
1:B:155:LYS:HD2	1:B:155:LYS:HA	1.89	0.41
1:C:190:ASN:OD1	1:C:229:LYS:HE2	2.21	0.41
1:D:60:ASP:HB2	1:D:334:GLY:HA2	2.03	0.41
1:E:109:ASP:C	1:E:109:ASP:OD1	2.64	0.41
1:B:429:GLU:OE2	1:B:434:VAL:HG11	2.21	0.40
1:A:223:ARG:HG3	1:A:289:LEU:HB2	2.02	0.40
1:A:171:HIS:CG	1:A:172:ALA:H	2.39	0.40
1:A:457:GLU:H	1:A:457:GLU:HG3	1.76	0.40
1:E:257:LYS:HA	1:E:260:LYS:CG	2.52	0.40
1:D:220:GLY:O	1:D:289:LEU:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	480/509 (94%)	468 (98%)	11 (2%)	1 (0%)	43 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	480/509 (94%)	465 (97%)	14 (3%)	1 (0%)	43	70
1	C	480/509 (94%)	463 (96%)	16 (3%)	1 (0%)	43	70
1	D	481/509 (94%)	469 (98%)	11 (2%)	1 (0%)	43	70
1	E	480/509 (94%)	465 (97%)	14 (3%)	1 (0%)	43	70
All	All	2401/2545 (94%)	2330 (97%)	66 (3%)	5 (0%)	43	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL
1	D	382	VAL
1	B	382	VAL
1	E	382	VAL
1	C	382	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	392/420 (93%)	391 (100%)	1 (0%)	86	84
1	B	397/420 (94%)	397 (100%)	0	100	100
1	C	398/420 (95%)	398 (100%)	0	100	100
1	D	397/420 (94%)	395 (100%)	2 (0%)	81	80
1	E	398/420 (95%)	398 (100%)	0	100	100
All	All	1982/2100 (94%)	1979 (100%)	3 (0%)	87	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	ASN
1	D	140	ASN
1	D	303	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	379	HIS
1	B	180	HIS
1	B	211	ASN
1	B	267	HIS
1	C	79	HIS
1	C	171	HIS
1	C	199	GLN
1	C	211	ASN
1	C	323	ASN
1	D	44	GLN
1	D	80	ASN
1	D	210	HIS
1	D	323	ASN
1	D	442	GLN
1	D	451	HIS
1	D	472	HIS
1	E	80	ASN
1	E	124	ASN
1	E	171	HIS
1	E	265	HIS
1	E	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

32 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	F	1	2,1	14,14,15	0.89	0	17,19,21	3.45	9 (52%)
2	NAG	F	2	2	14,14,15	0.78	0	17,19,21	0.90	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.78	0	17,19,21	1.08	2 (11%)
2	NAG	G	2	2	14,14,15	0.78	0	17,19,21	1.21	3 (17%)
3	NAG	H	1	3,1	14,14,15	0.76	0	17,19,21	1.45	4 (23%)
3	NAG	H	2	3	14,14,15	0.70	0	17,19,21	1.13	1 (5%)
3	BMA	H	3	3	11,11,12	0.94	0	15,15,17	1.98	5 (33%)
2	NAG	I	1	2,1	14,14,15	0.94	1 (7%)	17,19,21	3.05	7 (41%)
2	NAG	I	2	2	14,14,15	0.81	0	17,19,21	0.83	0
2	NAG	J	1	2,1	14,14,15	0.75	0	17,19,21	1.28	3 (17%)
2	NAG	J	2	2	14,14,15	0.73	0	17,19,21	1.03	1 (5%)
3	NAG	K	1	3,1	14,14,15	0.72	0	17,19,21	1.29	3 (17%)
3	NAG	K	2	3	14,14,15	0.73	0	17,19,21	0.96	0
3	BMA	K	3	3	11,11,12	0.90	0	15,15,17	2.69	6 (40%)
2	NAG	L	1	2,1	14,14,15	0.62	0	17,19,21	3.45	6 (35%)
2	NAG	L	2	2	14,14,15	0.66	0	17,19,21	3.15	9 (52%)
2	NAG	M	1	2,1	14,14,15	0.76	0	17,19,21	1.72	4 (23%)
2	NAG	M	2	2	14,14,15	0.67	0	17,19,21	0.98	1 (5%)
2	NAG	N	1	2,1	14,14,15	0.92	1 (7%)	17,19,21	1.06	1 (5%)
2	NAG	N	2	2	14,14,15	0.72	0	17,19,21	1.11	1 (5%)
2	NAG	O	1	2,1	14,14,15	0.96	1 (7%)	17,19,21	3.11	9 (52%)
2	NAG	O	2	2	14,14,15	0.80	0	17,19,21	1.54	2 (11%)
2	NAG	P	1	2,1	14,14,15	0.76	0	17,19,21	1.12	3 (17%)
2	NAG	P	2	2	14,14,15	0.72	0	17,19,21	1.04	1 (5%)
3	NAG	Q	1	3,1	14,14,15	0.76	0	17,19,21	1.65	4 (23%)
3	NAG	Q	2	3	14,14,15	0.73	0	17,19,21	1.64	5 (29%)
3	BMA	Q	3	3	11,11,12	0.93	0	15,15,17	2.19	5 (33%)
2	NAG	R	1	2,1	14,14,15	0.96	1 (7%)	17,19,21	3.24	8 (47%)
2	NAG	R	2	2	14,14,15	0.77	0	17,19,21	0.78	0
3	NAG	S	1	3,1	14,14,15	0.75	0	17,19,21	2.71	4 (23%)
3	NAG	S	2	3	14,14,15	0.67	0	17,19,21	1.28	4 (23%)
3	BMA	S	3	3	11,11,12	0.92	1 (9%)	15,15,17	2.27	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	1/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	1/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	1/2/19/22	0/1/1/1
2	NAG	R	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	1/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	BMA	S	3	3	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	NAG	C1-C2	2.31	1.55	1.52
2	O	1	NAG	C1-C2	2.27	1.55	1.52
2	R	1	NAG	C1-C2	2.13	1.55	1.52
2	N	1	NAG	O5-C1	-2.05	1.40	1.43
3	S	3	BMA	C2-C3	2.04	1.55	1.52

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	1	NAG	C2-N2-C7	9.16	135.17	122.90
2	F	1	NAG	C2-N2-C7	-8.83	111.07	122.90
2	R	1	NAG	C2-N2-C7	-8.60	111.38	122.90
2	L	2	NAG	C1-O5-C5	8.55	123.65	112.19
2	I	1	NAG	C2-N2-C7	-8.54	111.46	122.90
2	O	1	NAG	C2-N2-C7	-7.93	112.27	122.90
3	K	3	BMA	C1-O5-C5	7.65	122.43	112.19
2	L	1	NAG	C2-N2-C7	7.49	132.94	122.90
2	L	1	NAG	C4-C3-C2	7.04	121.33	111.02
3	S	3	BMA	C1-O5-C5	6.40	120.76	112.19
2	F	1	NAG	O5-C1-C2	5.69	120.09	111.29
2	R	1	NAG	C1-O5-C5	5.32	119.32	112.19
3	Q	3	BMA	C1-O5-C5	5.25	119.22	112.19
2	L	1	NAG	O5-C1-C2	-5.22	103.22	111.29
2	F	1	NAG	C1-O5-C5	5.20	119.16	112.19
2	I	1	NAG	C1-O5-C5	5.10	119.02	112.19
2	L	1	NAG	O4-C4-C3	-4.84	98.96	110.38
2	O	2	NAG	C2-N2-C7	4.84	129.38	122.90
2	L	2	NAG	C4-C3-C2	4.82	118.08	111.02
2	O	1	NAG	C1-O5-C5	4.80	118.62	112.19
2	L	2	NAG	O4-C4-C3	-4.78	99.11	110.38
2	R	1	NAG	O5-C1-C2	4.62	118.44	111.29
2	L	1	NAG	O4-C4-C5	4.42	120.20	109.32
2	O	1	NAG	C4-C3-C2	4.34	117.38	111.02
2	L	1	NAG	C1-O5-C5	4.32	117.98	112.19
2	I	1	NAG	O5-C1-C2	4.29	117.93	111.29
3	Q	2	NAG	C2-N2-C7	4.04	128.31	122.90
3	K	3	BMA	C3-C4-C5	3.94	117.37	110.23
2	M	1	NAG	C2-N2-C7	3.83	128.03	122.90
3	H	3	BMA	C3-C4-C5	3.73	116.99	110.23
3	Q	3	BMA	C3-C4-C5	3.69	116.92	110.23
3	H	3	BMA	C1-O5-C5	3.65	117.08	112.19
2	F	1	NAG	O4-C4-C3	-3.62	101.85	110.38
3	K	3	BMA	C2-C3-C4	3.52	117.05	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-C2-N2	-3.51	104.90	110.43
2	O	1	NAG	O4-C4-C3	-3.49	102.16	110.38
2	O	1	NAG	O5-C1-C2	3.47	116.67	111.29
2	R	1	NAG	C4-C3-C2	3.47	116.10	111.02
3	S	1	NAG	C1-C2-N2	3.46	115.89	110.43
2	F	1	NAG	C4-C3-C2	3.44	116.06	111.02
2	M	1	NAG	O4-C4-C3	-3.39	102.38	110.38
2	L	2	NAG	C2-N2-C7	3.38	127.43	122.90
2	R	1	NAG	O4-C4-C3	-3.35	102.49	110.38
3	Q	1	NAG	O4-C4-C3	-3.33	102.53	110.38
3	Q	3	BMA	C2-C3-C4	3.25	116.57	110.86
2	I	1	NAG	C4-C3-C2	3.19	115.70	111.02
2	L	2	NAG	O4-C4-C5	3.18	117.16	109.32
3	S	1	NAG	O7-C7-N2	3.01	127.30	121.98
3	K	1	NAG	C1-O5-C5	2.98	116.18	112.19
3	S	3	BMA	C2-C3-C4	2.96	116.07	110.86
2	I	1	NAG	C3-C4-C5	2.91	115.51	110.23
2	M	2	NAG	O5-C1-C2	-2.91	106.79	111.29
3	H	3	BMA	C2-C3-C4	2.89	115.94	110.86
2	L	2	NAG	O5-C5-C6	-2.88	102.05	107.66
2	F	1	NAG	O5-C5-C6	-2.88	102.06	107.66
2	J	1	NAG	O4-C4-C3	-2.88	103.59	110.38
2	P	2	NAG	O5-C1-C2	-2.80	106.96	111.29
2	R	1	NAG	C1-C2-N2	-2.75	106.10	110.43
2	G	2	NAG	O5-C1-C2	-2.74	107.06	111.29
3	S	1	NAG	O5-C1-C2	-2.68	107.15	111.29
2	O	1	NAG	C8-C7-N2	2.66	120.53	116.12
3	Q	1	NAG	C1-O5-C5	2.64	115.73	112.19
3	Q	1	NAG	O5-C1-C2	-2.63	107.23	111.29
2	I	1	NAG	O4-C4-C3	-2.62	104.20	110.38
2	F	1	NAG	C8-C7-N2	2.62	120.46	116.12
3	S	3	BMA	C1-C2-C3	2.58	113.40	109.64
2	J	2	NAG	O5-C1-C2	-2.58	107.30	111.29
2	L	2	NAG	C3-C4-C5	-2.55	105.61	110.23
2	R	1	NAG	C3-C4-C5	2.54	114.84	110.23
2	N	2	NAG	C2-N2-C7	2.53	126.29	122.90
3	H	1	NAG	C1-O5-C5	2.52	115.56	112.19
2	I	1	NAG	C8-C7-N2	2.51	120.28	116.12
3	H	3	BMA	O3-C3-C2	-2.49	104.97	110.05
3	K	1	NAG	O5-C1-C2	-2.48	107.46	111.29
2	O	1	NAG	C1-C2-N2	-2.48	106.53	110.43
2	O	1	NAG	O4-C4-C5	2.48	115.42	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1	NAG	C1-O5-C5	2.47	115.50	112.19
2	J	1	NAG	O5-C1-C2	-2.45	107.50	111.29
2	L	2	NAG	O5-C5-C4	-2.45	104.88	110.83
3	H	2	NAG	O4-C4-C3	-2.44	104.63	110.38
3	H	1	NAG	O4-C4-C3	-2.44	104.63	110.38
3	Q	2	NAG	O4-C4-C3	-2.41	104.69	110.38
3	S	2	NAG	O5-C1-C2	-2.40	107.58	111.29
2	R	1	NAG	C8-C7-N2	2.39	120.09	116.12
2	O	2	NAG	C1-O5-C5	2.36	115.36	112.19
3	H	3	BMA	O4-C4-C3	-2.36	104.82	110.38
2	F	1	NAG	C3-C4-C5	2.36	114.50	110.23
3	K	3	BMA	O5-C5-C4	2.35	116.54	110.83
2	M	1	NAG	C1-O5-C5	-2.34	109.05	112.19
3	S	3	BMA	O4-C4-C3	-2.34	104.86	110.38
3	H	1	NAG	C1-C2-N2	2.34	114.11	110.43
3	Q	1	NAG	C2-N2-C7	2.33	126.02	122.90
3	H	1	NAG	O5-C1-C2	-2.31	107.71	111.29
2	G	2	NAG	C2-N2-C7	2.31	125.99	122.90
3	Q	3	BMA	O3-C3-C2	-2.30	105.35	110.05
2	L	2	NAG	C6-C5-C4	2.30	118.67	113.02
3	S	2	NAG	O4-C4-C3	-2.30	104.96	110.38
3	Q	3	BMA	O4-C4-C3	-2.29	104.98	110.38
2	P	1	NAG	C1-O5-C5	-2.29	109.12	112.19
3	Q	2	NAG	O5-C1-C2	-2.26	107.79	111.29
3	K	3	BMA	O3-C3-C2	-2.26	105.44	110.05
2	G	1	NAG	C1-O5-C5	-2.25	109.17	112.19
3	K	3	BMA	O4-C4-C3	-2.22	105.15	110.38
2	P	1	NAG	O4-C4-C3	-2.20	105.20	110.38
3	S	2	NAG	C2-N2-C7	2.19	125.83	122.90
2	M	1	NAG	O5-C1-C2	-2.17	107.93	111.29
2	O	1	NAG	O5-C5-C6	-2.13	103.52	107.66
3	Q	2	NAG	O4-C4-C5	2.12	114.54	109.32
2	J	1	NAG	C1-O5-C5	-2.10	109.38	112.19
2	P	1	NAG	C3-C4-C5	2.09	114.02	110.23
3	K	1	NAG	O4-C4-C3	-2.08	105.48	110.38
3	Q	2	NAG	C1-C2-N2	-2.06	107.18	110.43
3	S	2	NAG	C1-O5-C5	2.06	114.94	112.19
2	F	2	NAG	O5-C1-C2	-2.02	108.16	111.29
2	G	1	NAG	O5-C1-C2	-2.02	108.17	111.29
2	G	2	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	1	NAG	C1-C2-N2-C7
2	J	2	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	S	3	BMA	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
3	S	3	BMA	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
3	Q	3	BMA	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6

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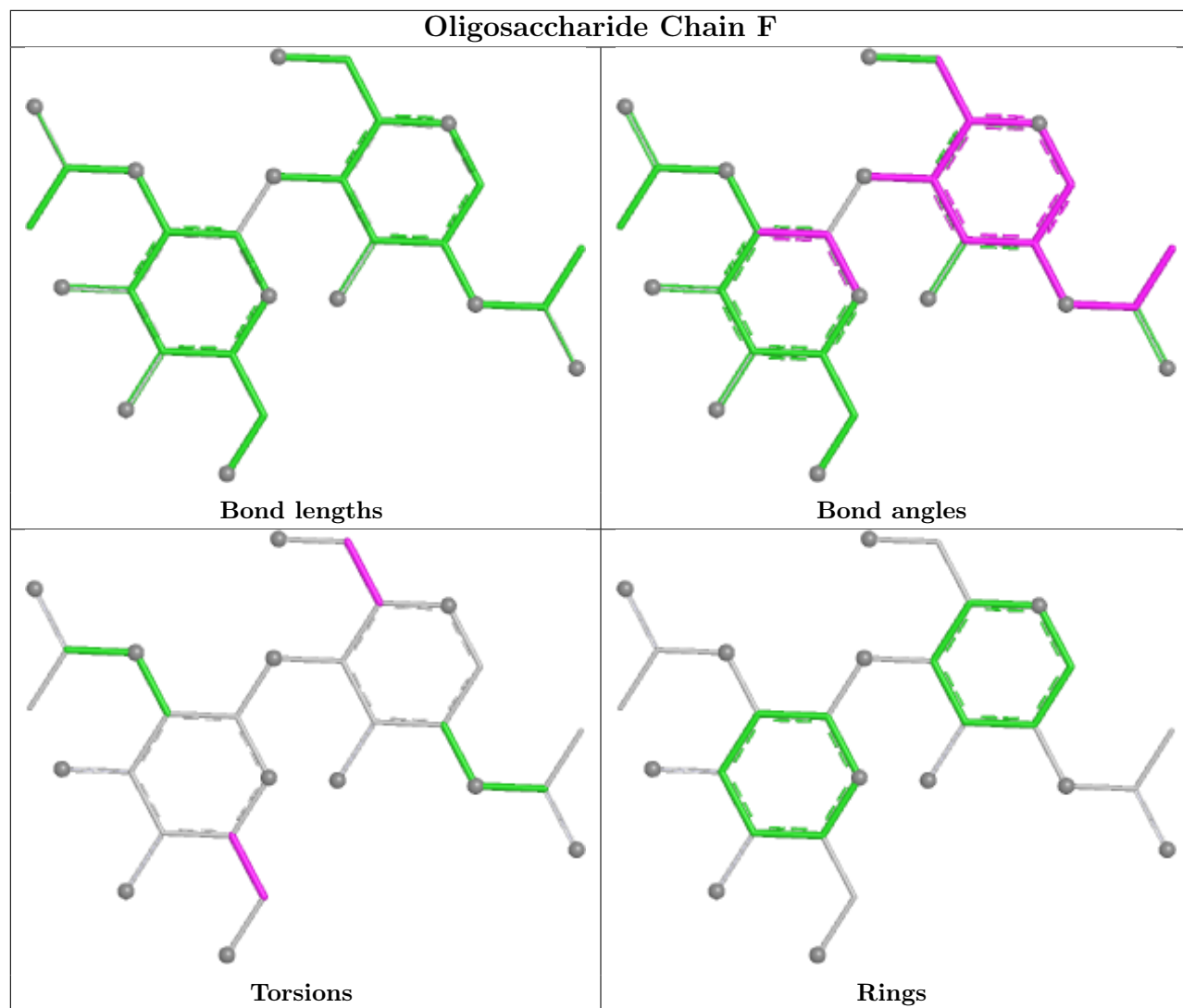
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6

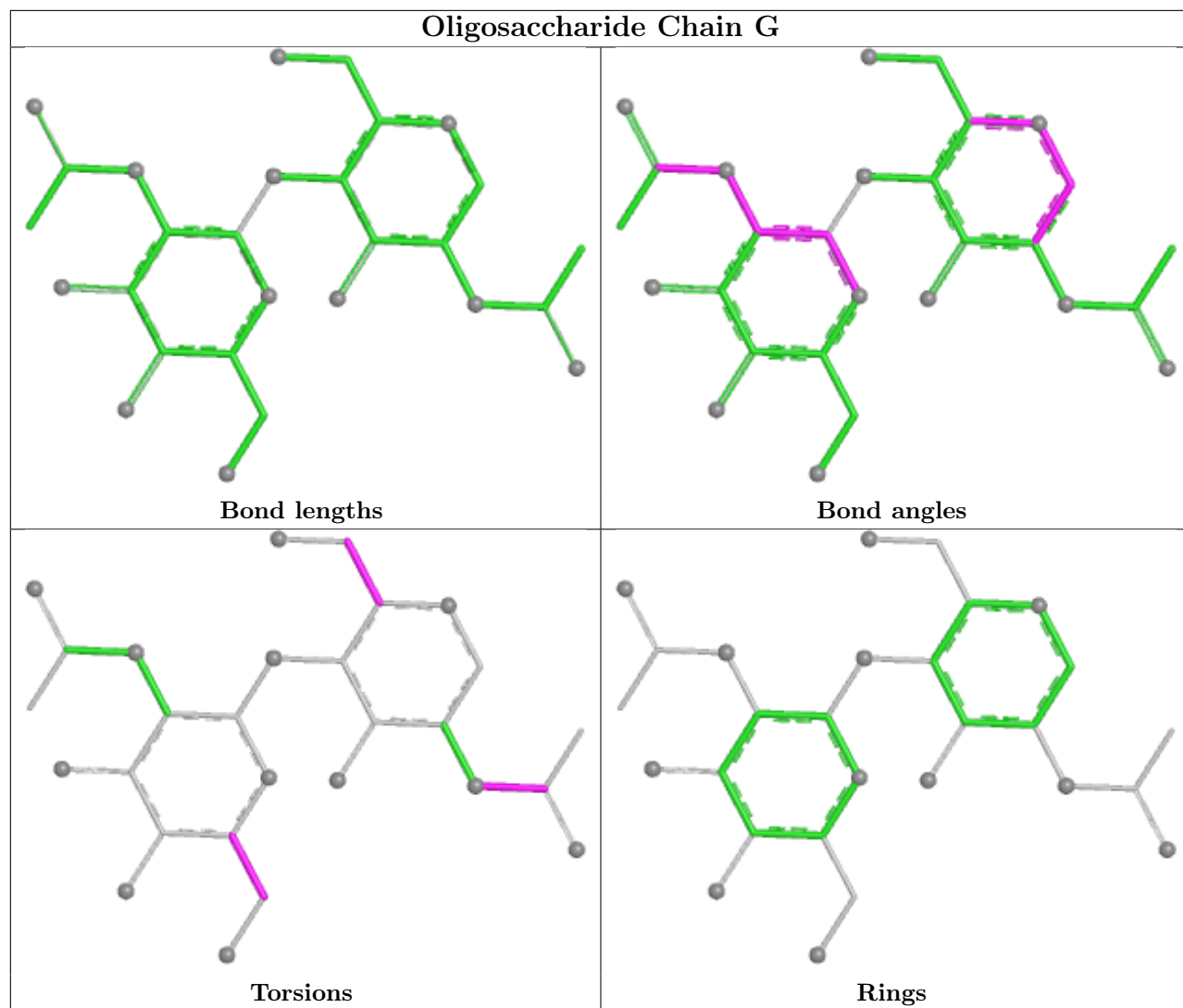
There are no ring outliers.

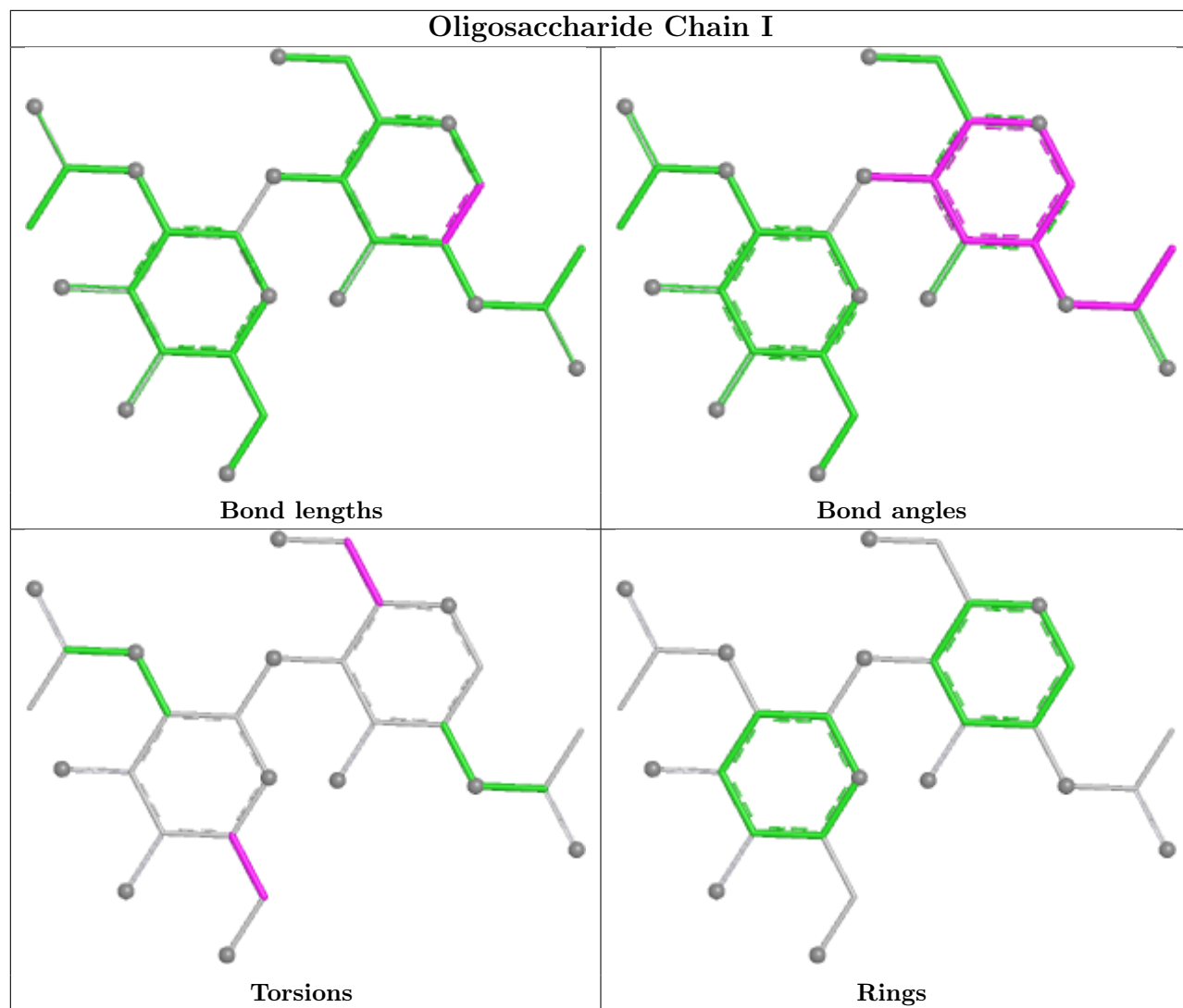
7 monomers are involved in 8 short contacts:

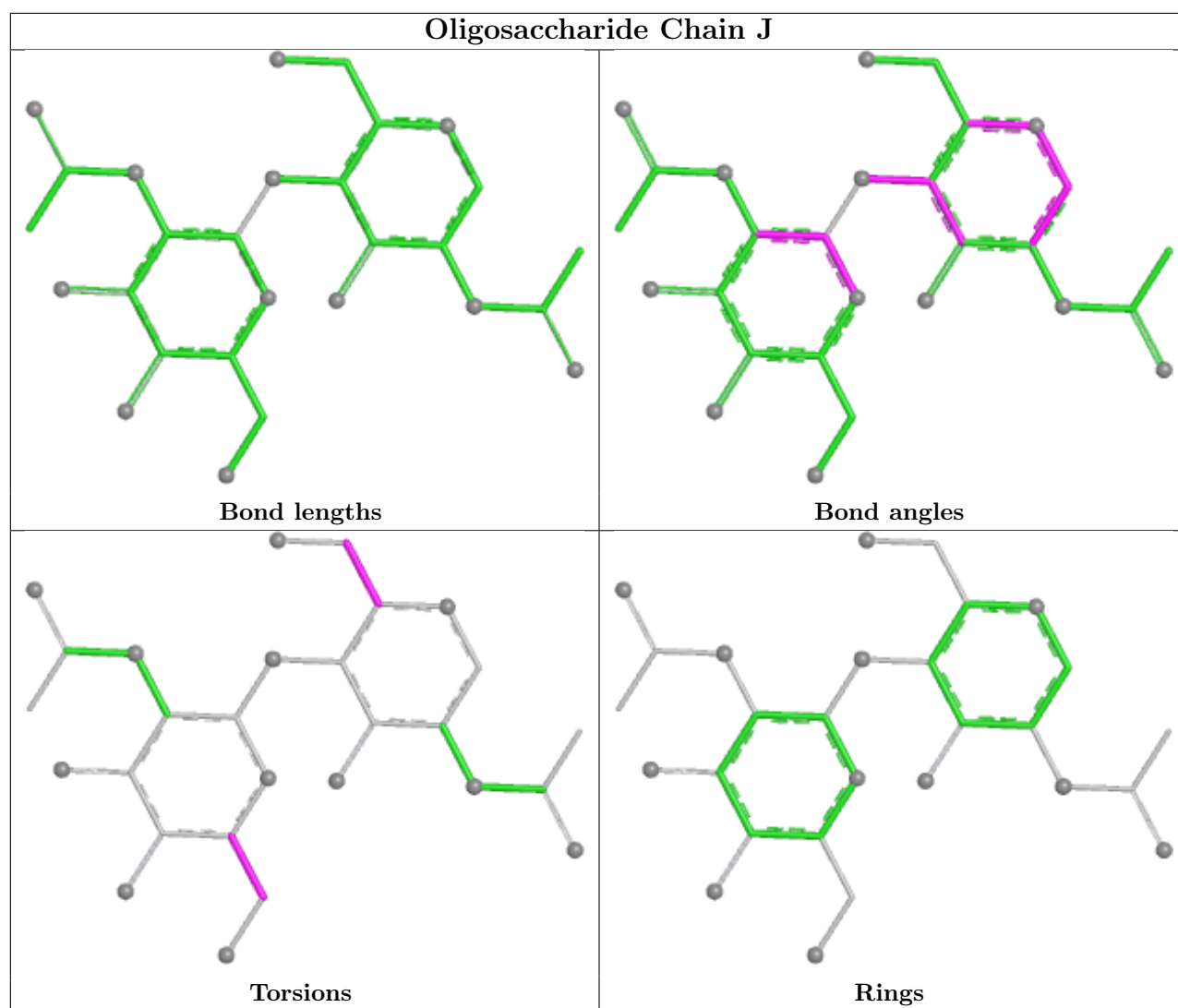
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	NAG	2	0
2	F	1	NAG	1	0
2	R	1	NAG	1	0
3	Q	1	NAG	1	0
2	O	2	NAG	1	0
2	I	1	NAG	1	0
2	L	1	NAG	2	0

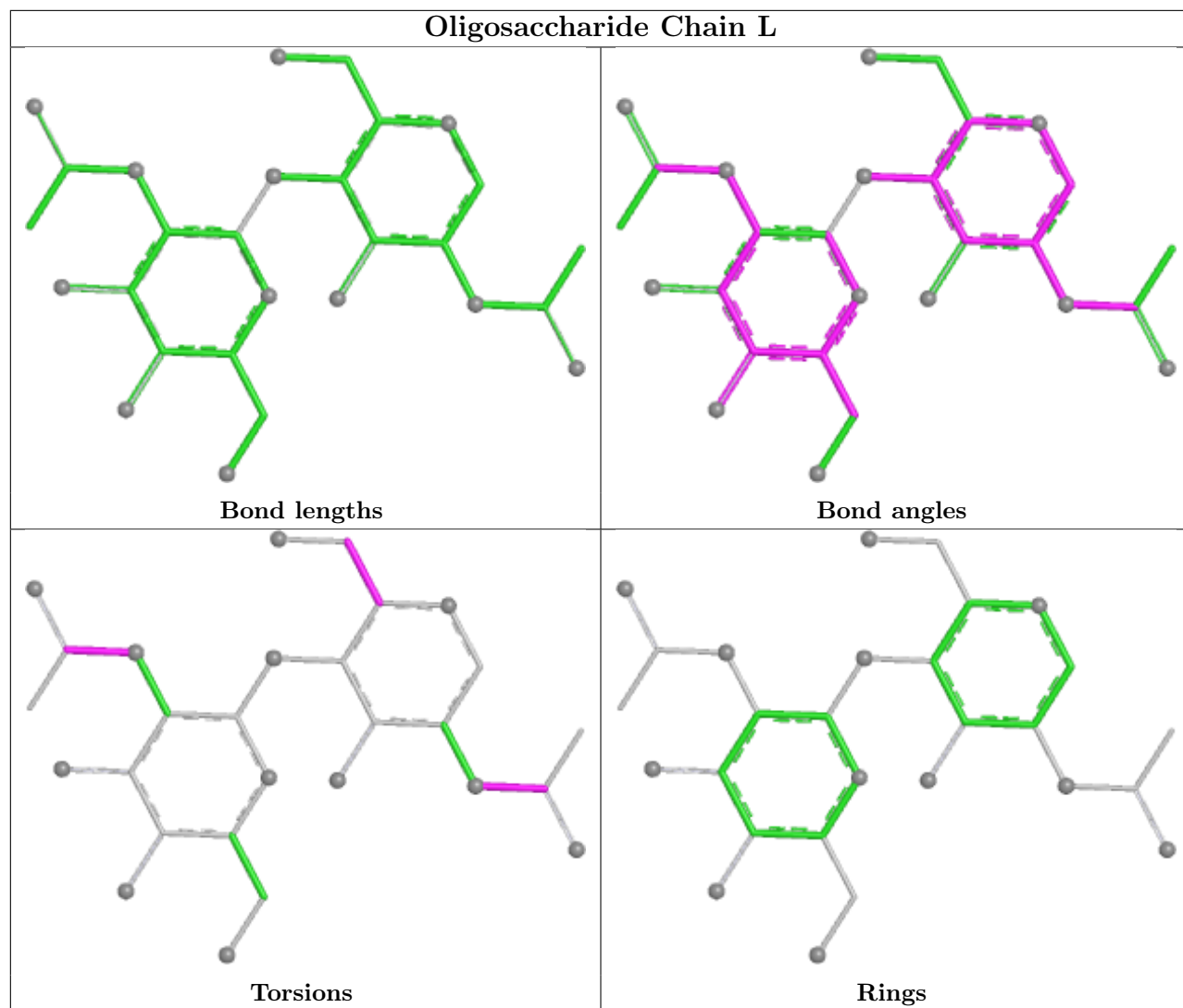
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

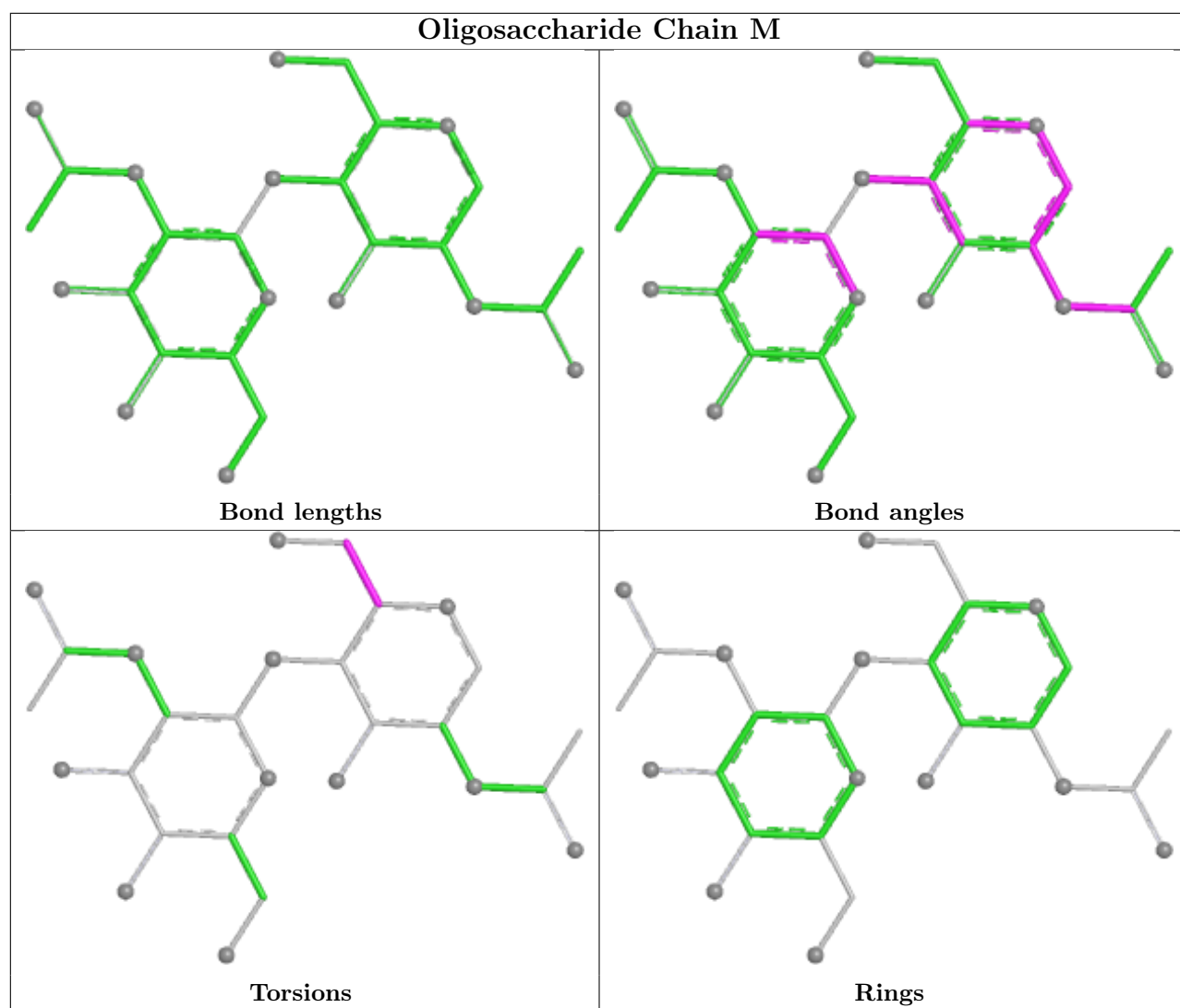


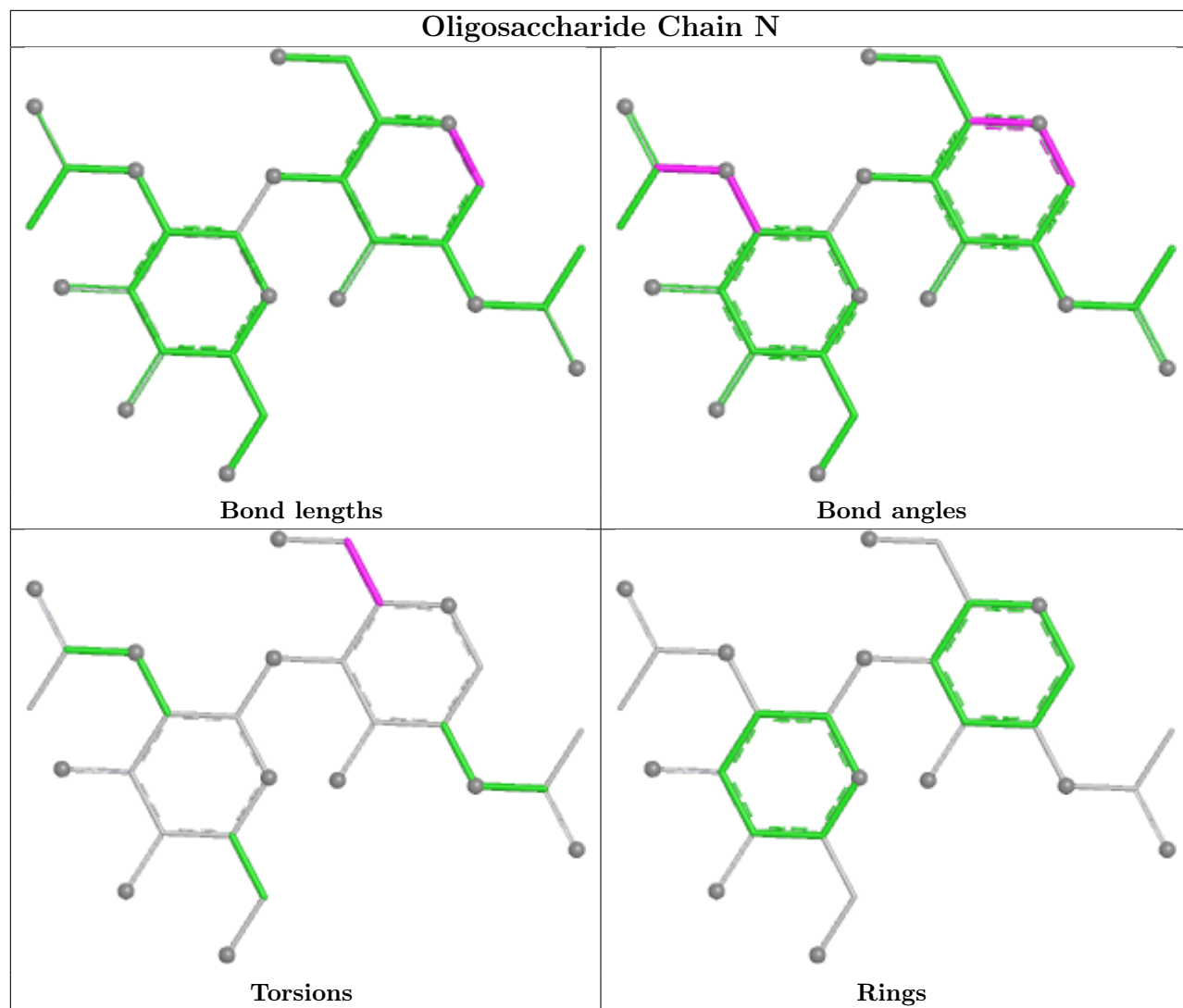


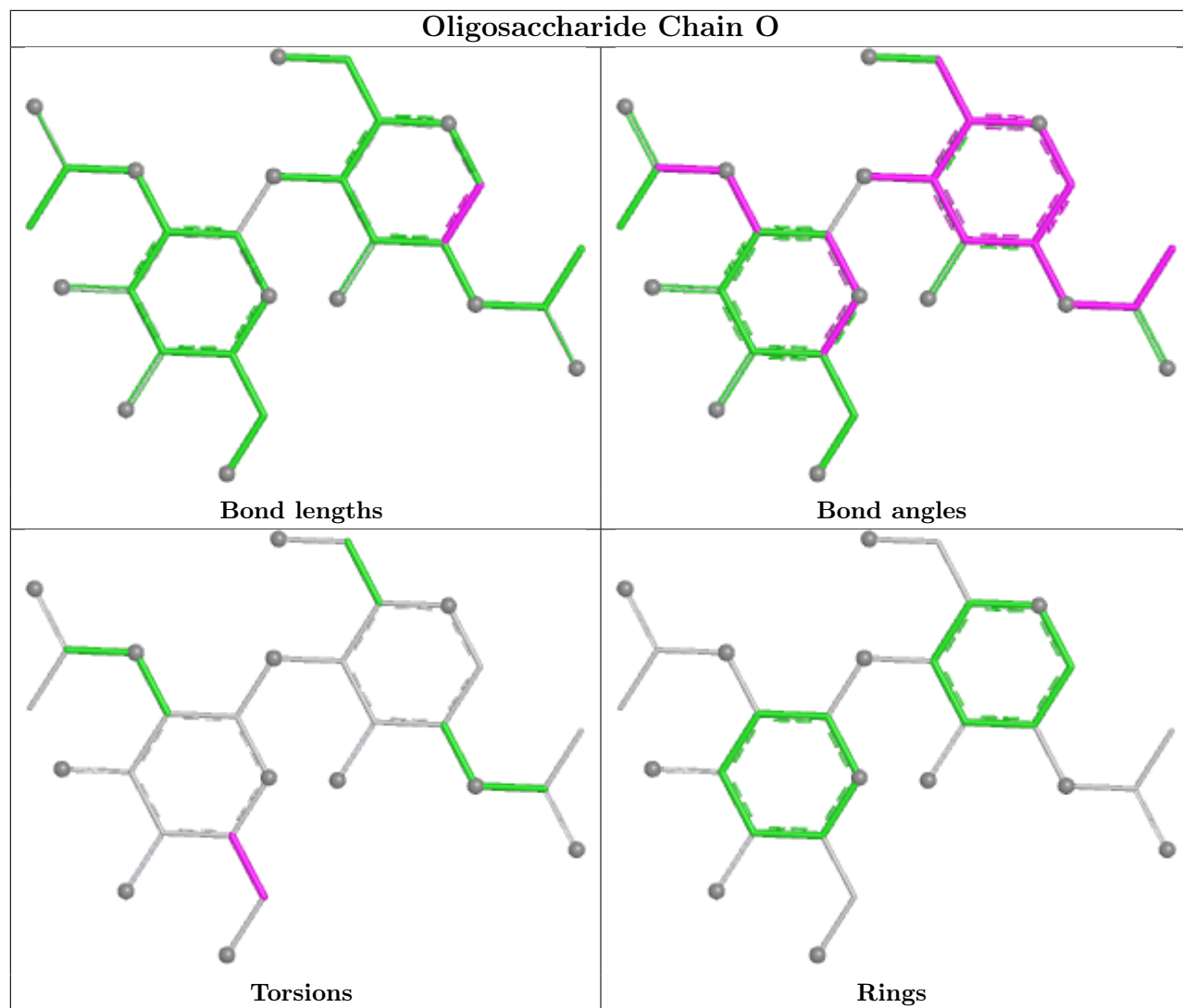


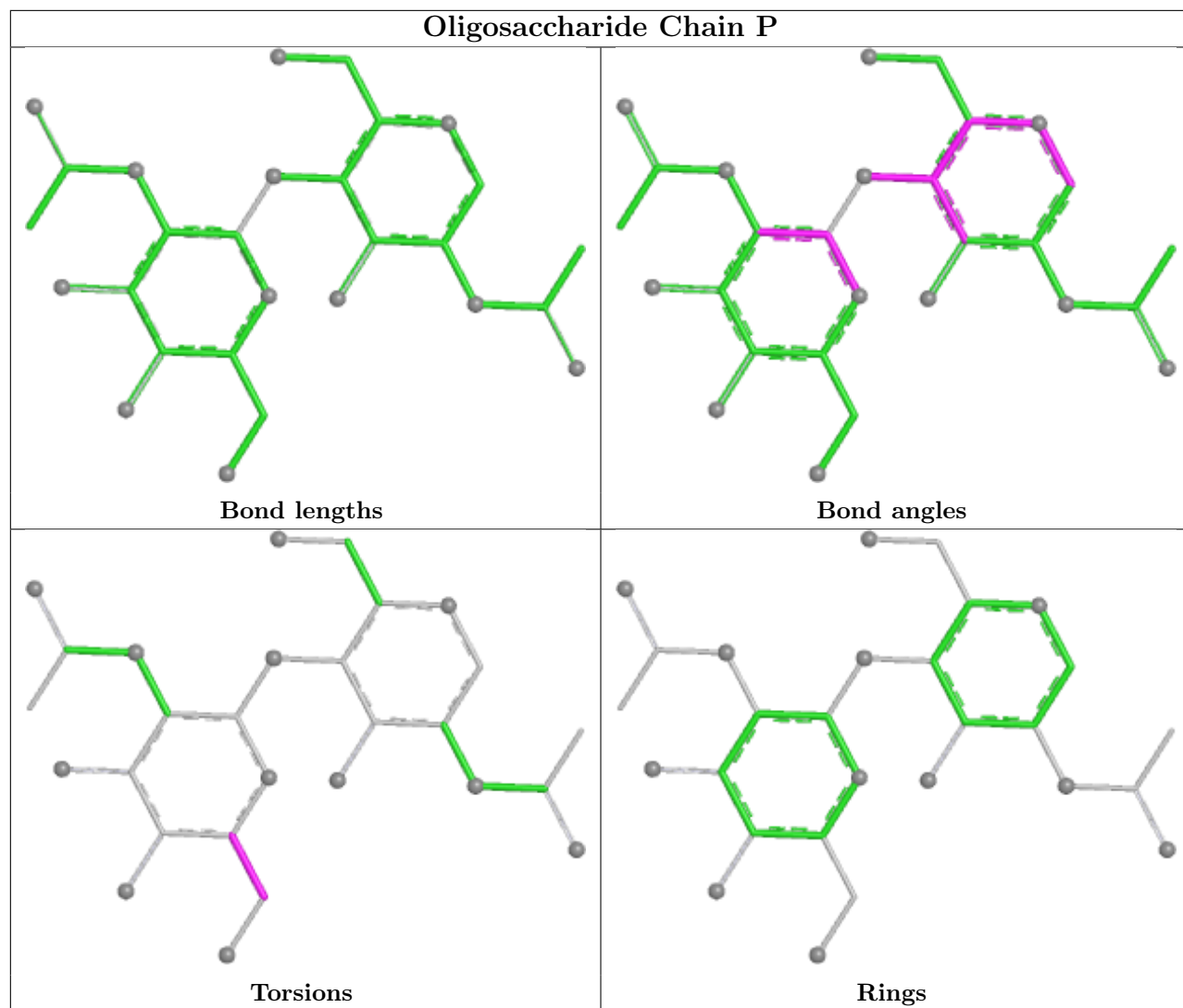


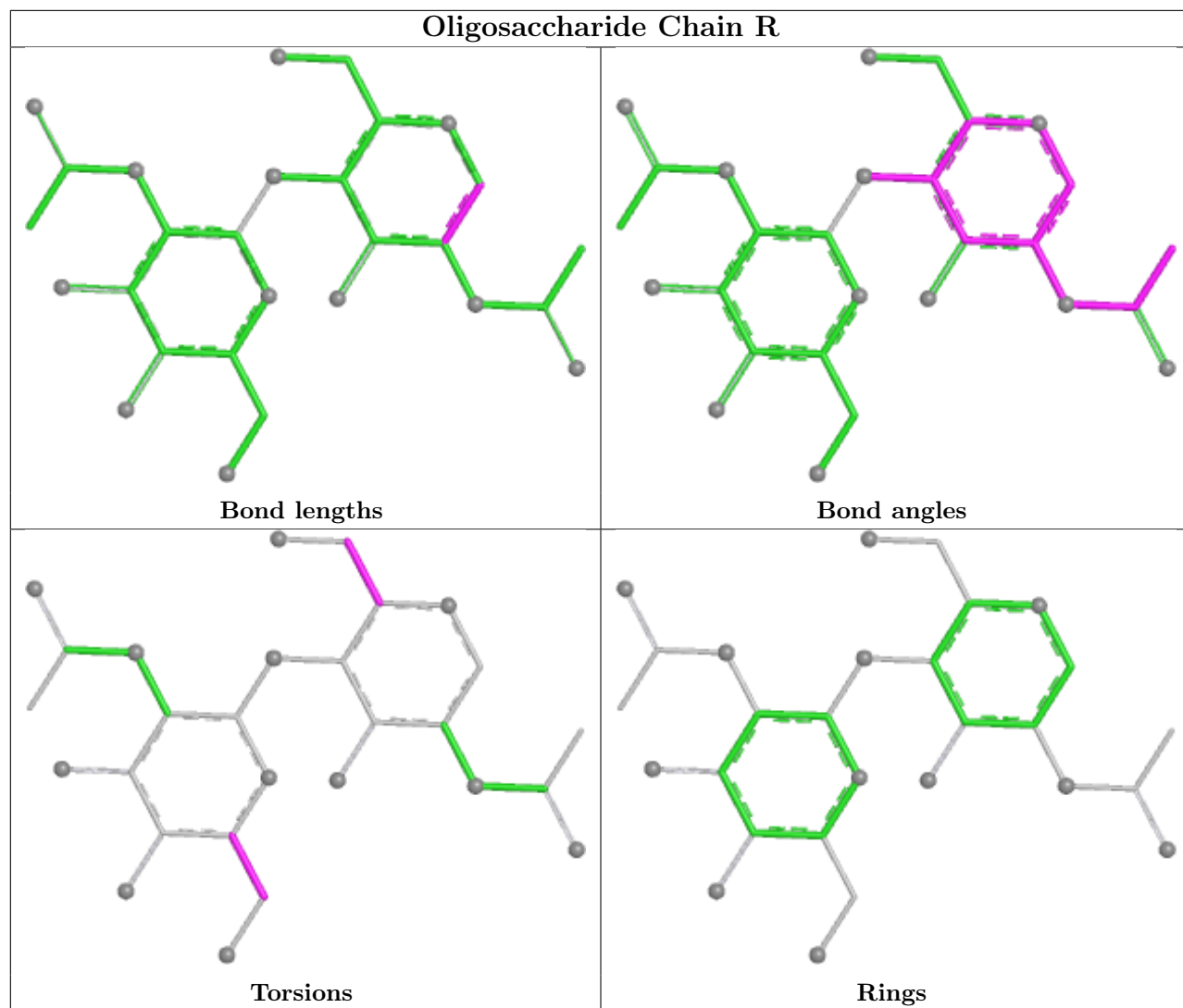


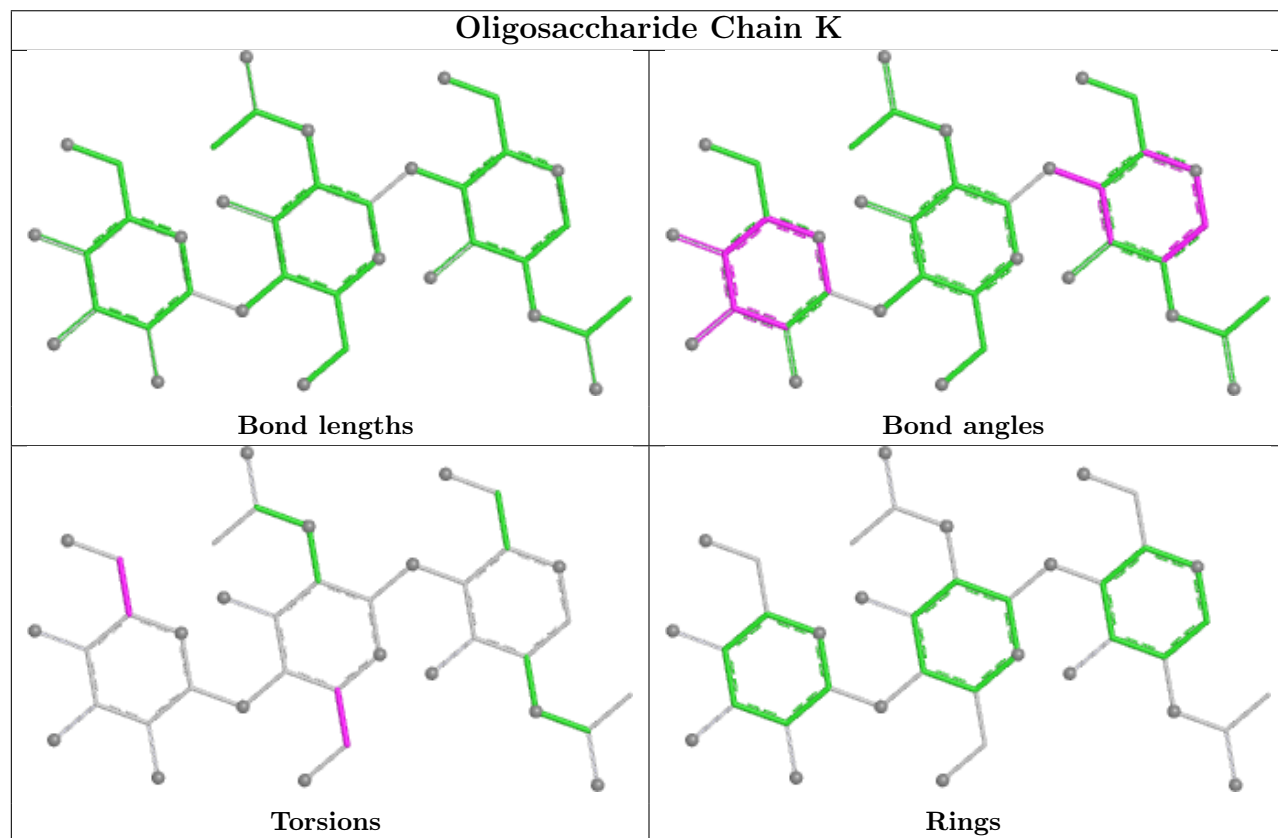
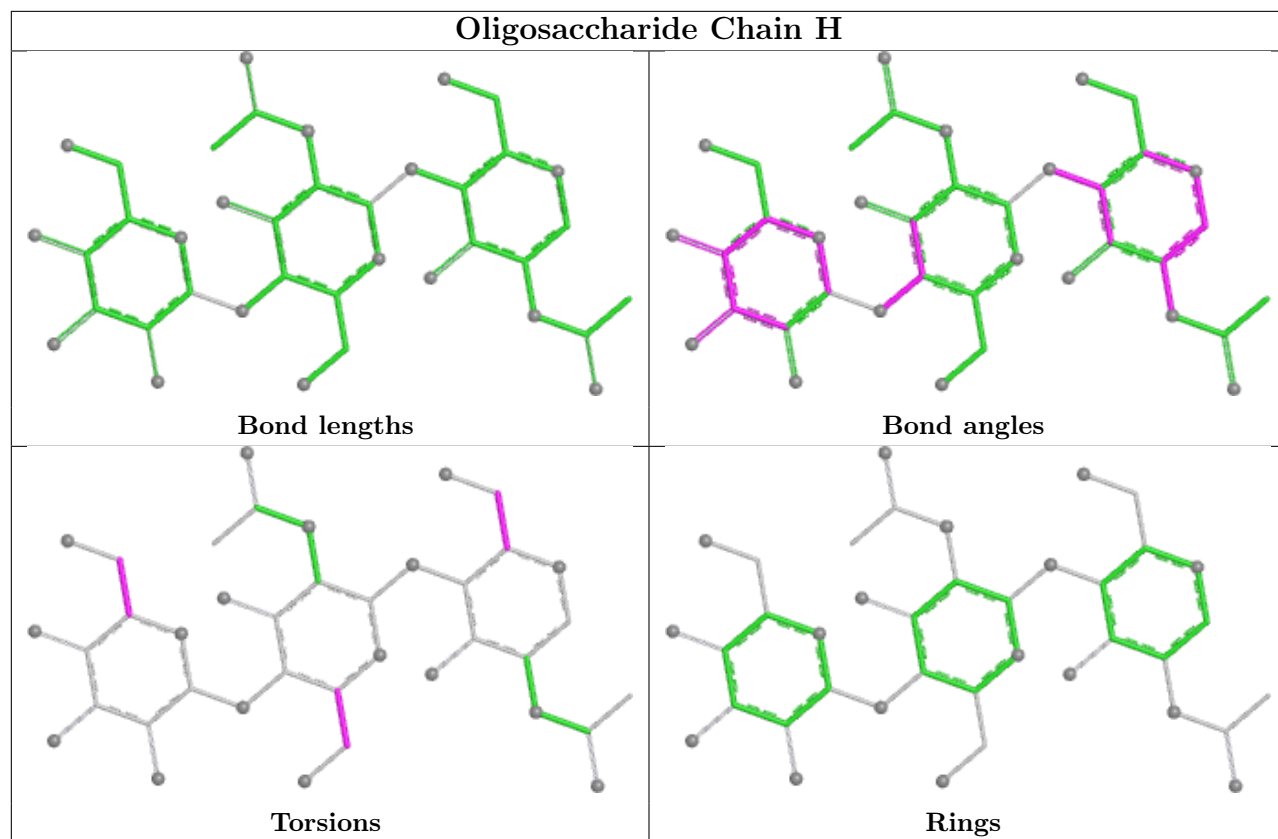


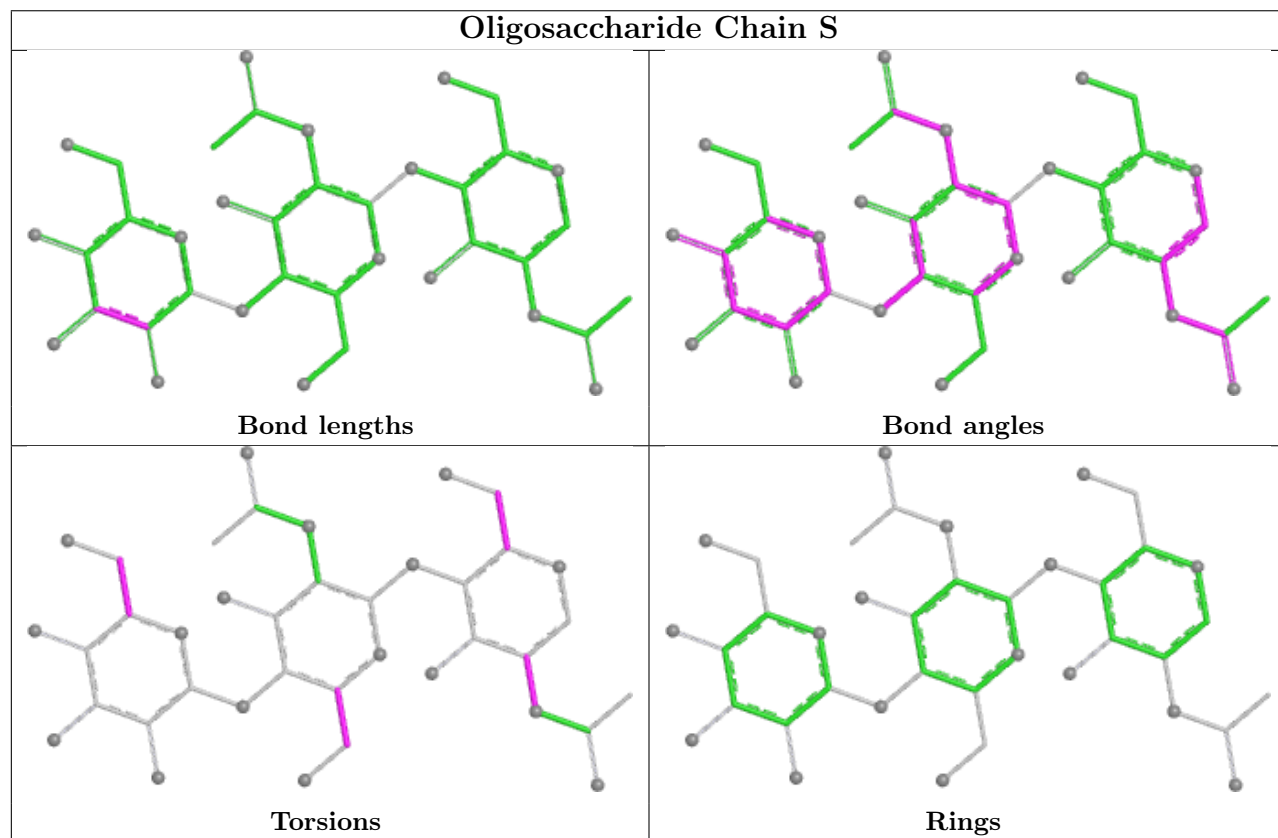
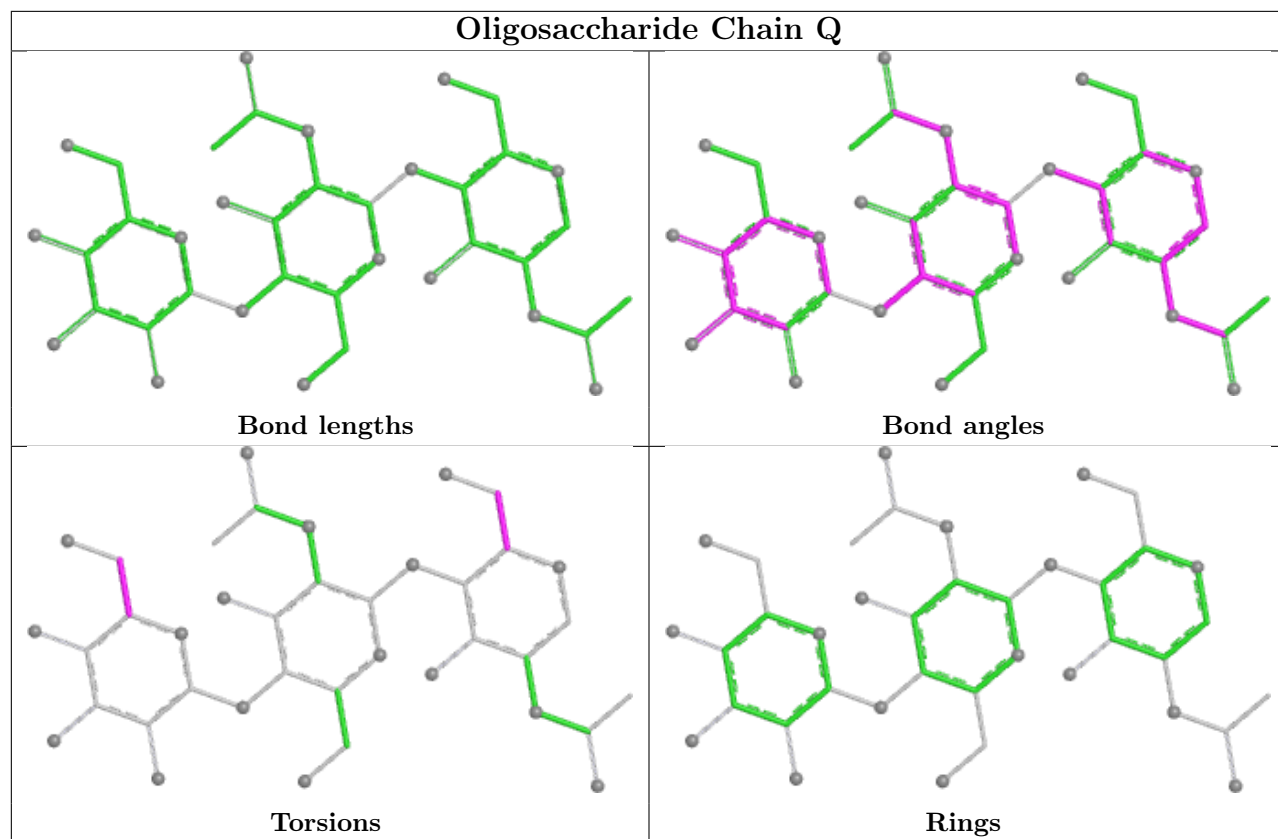












5.6 Ligand geometry

Of 31 ligands modelled in this entry, 20 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	605	1	14,14,15	0.65	0	17,19,21	0.84	0
8	PO4	D	606	-	4,4,4	1.52	1 (25%)	6,6,6	0.49	0
7	NAG	B	605	1	14,14,15	0.59	0	17,19,21	3.61	7 (41%)
8	PO4	C	606	4	4,4,4	1.27	0	6,6,6	0.62	0
8	PO4	E	607	-	4,4,4	1.54	1 (25%)	6,6,6	0.46	0
8	PO4	A	606	-	4,4,4	1.49	1 (25%)	6,6,6	0.77	0
8	PO4	B	606	-	4,4,4	1.52	1 (25%)	6,6,6	0.48	0
7	NAG	D	605	1	14,14,15	0.85	1 (7%)	17,19,21	1.69	4 (23%)
7	NAG	A	605	1	14,14,15	0.54	0	17,19,21	4.17	10 (58%)
7	NAG	E	606	1	14,14,15	0.74	0	17,19,21	1.16	2 (11%)
7	NAG	E	605	1	14,14,15	0.28	0	17,19,21	1.17	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	605	1	-	1/6/23/26	0/1/1/1
7	NAG	B	605	1	-	2/6/23/26	0/1/1/1
7	NAG	D	605	1	-	0/6/23/26	0/1/1/1
7	NAG	A	605	1	-	2/6/23/26	0/1/1/1
7	NAG	E	606	1	-	2/6/23/26	0/1/1/1
7	NAG	E	605	1	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	607	PO4	P-O1	2.73	1.57	1.50
8	D	606	PO4	P-O1	2.66	1.56	1.50
8	B	606	PO4	P-O1	2.66	1.56	1.50
8	A	606	PO4	P-O1	2.55	1.56	1.50
7	D	605	NAG	C1-C2	2.23	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	605	NAG	C1-O5-C5	8.77	123.94	112.19
7	A	605	NAG	C1-O5-C5	8.46	123.53	112.19
7	A	605	NAG	O5-C1-C2	8.01	123.69	111.29
7	A	605	NAG	C2-N2-C7	7.14	132.46	122.90
7	B	605	NAG	O5-C1-C2	6.15	120.81	111.29
7	A	605	NAG	C3-C4-C5	5.86	120.86	110.23
7	A	605	NAG	C4-C3-C2	5.05	118.42	111.02
7	B	605	NAG	C4-C3-C2	4.80	118.05	111.02
7	B	605	NAG	C3-C4-C5	4.80	118.93	110.23
7	D	605	NAG	C1-O5-C5	4.69	118.47	112.19
7	B	605	NAG	C1-C2-N2	-4.45	103.43	110.43
7	B	605	NAG	O4-C4-C3	-3.84	101.31	110.38
7	A	605	NAG	C1-C2-N2	-3.78	104.47	110.43
7	E	605	NAG	C1-O5-C5	3.40	116.75	112.19
7	B	605	NAG	O5-C5-C4	3.27	118.78	110.83
7	A	605	NAG	O4-C4-C3	-3.22	102.79	110.38
7	E	606	NAG	O5-C1-C2	-2.42	107.55	111.29
7	A	605	NAG	O5-C5-C4	2.40	116.67	110.83
7	D	605	NAG	C3-C4-C5	2.19	114.19	110.23
7	A	605	NAG	O7-C7-N2	2.17	125.82	121.98
7	E	606	NAG	O4-C4-C3	-2.16	105.28	110.38
7	D	605	NAG	C2-N2-C7	2.09	125.70	122.90
7	A	605	NAG	C6-C5-C4	-2.09	107.89	113.02
7	D	605	NAG	C4-C3-C2	2.03	114.00	111.02

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	605	NAG	C1-C2-N2-C7
7	E	605	NAG	C8-C7-N2-C2
7	E	605	NAG	O7-C7-N2-C2
7	B	605	NAG	O5-C5-C6-O6

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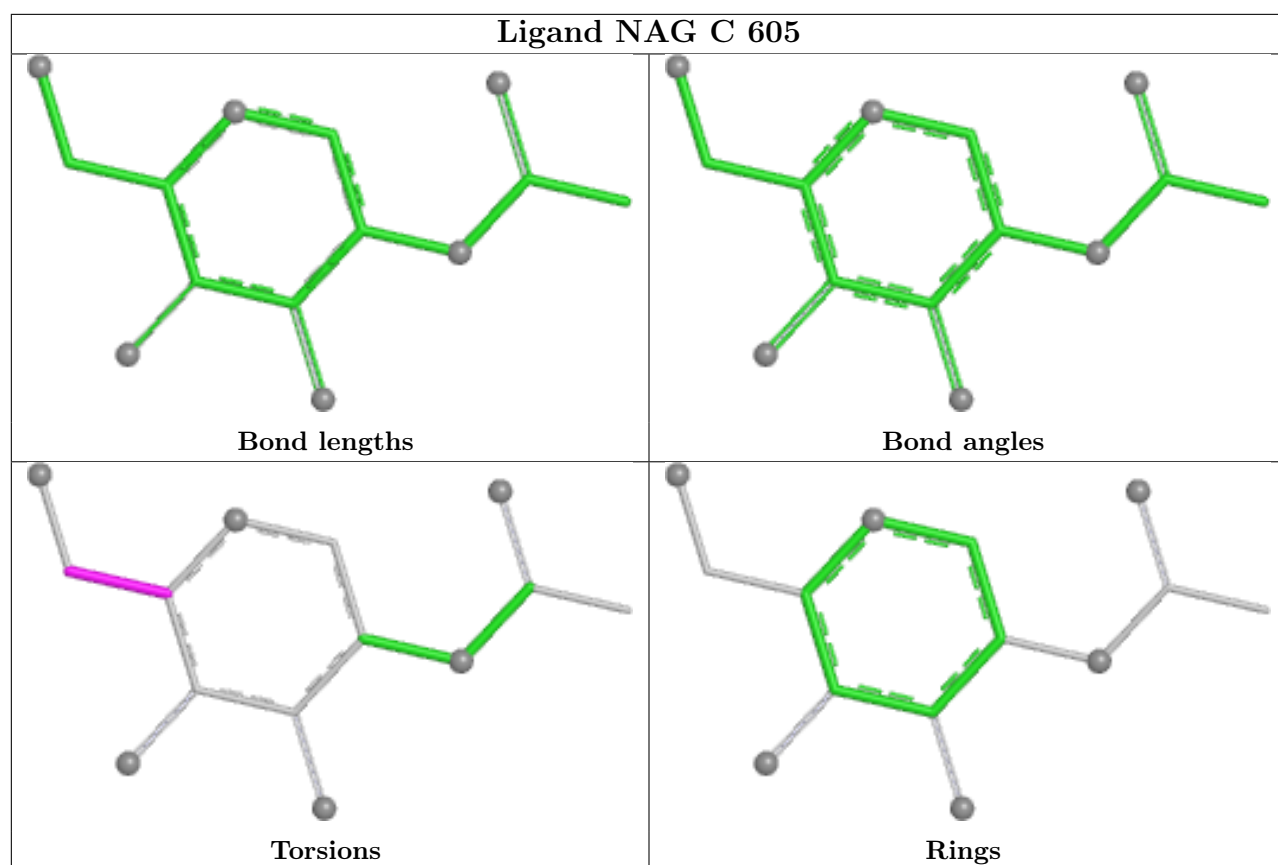
Mol	Chain	Res	Type	Atoms
7	E	606	NAG	C8-C7-N2-C2
7	E	606	NAG	O7-C7-N2-C2
7	B	605	NAG	C4-C5-C6-O6
7	C	605	NAG	O5-C5-C6-O6
7	A	605	NAG	C1-C2-N2-C7
7	E	605	NAG	C4-C5-C6-O6
7	A	605	NAG	C3-C2-N2-C7

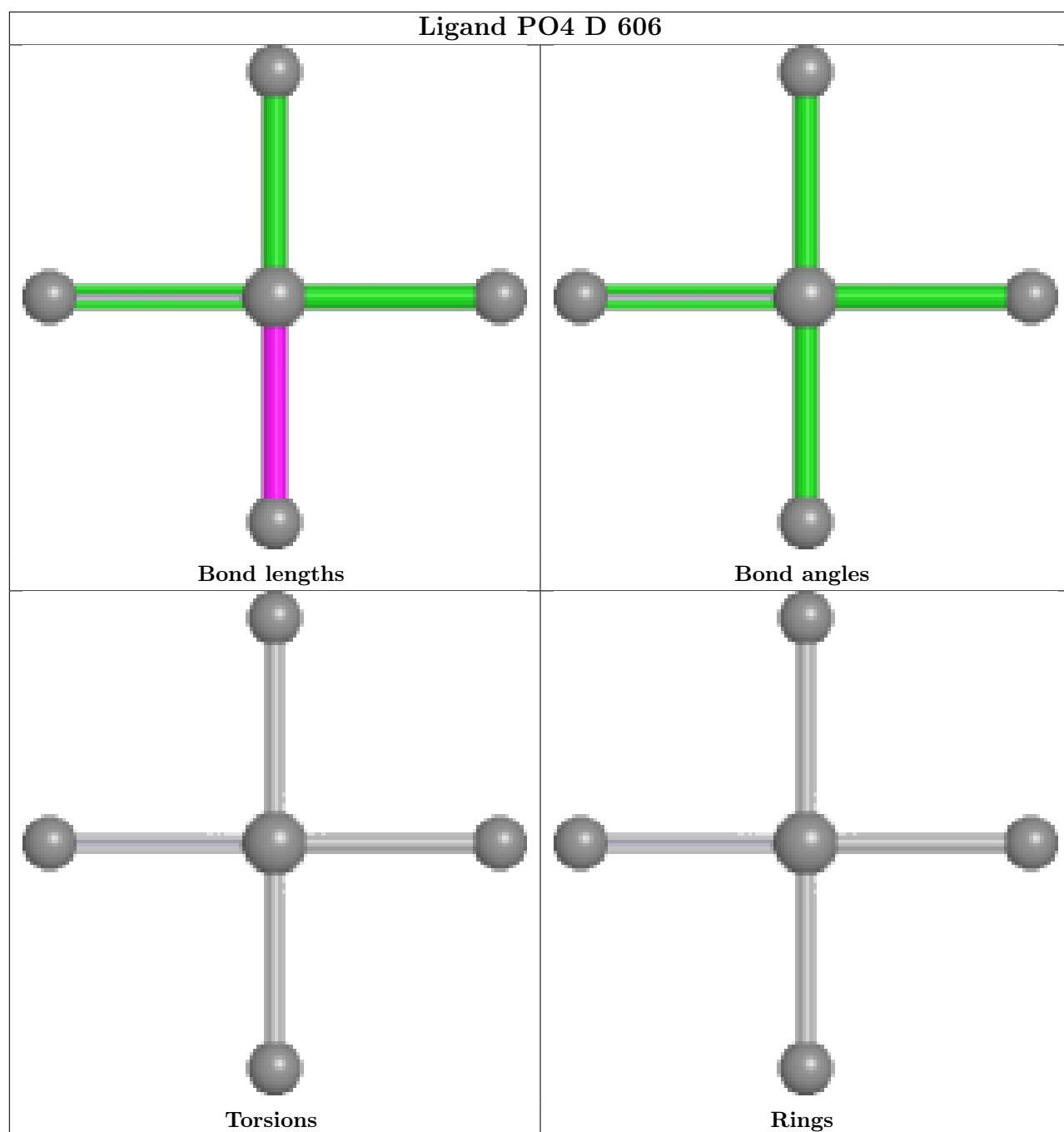
There are no ring outliers.

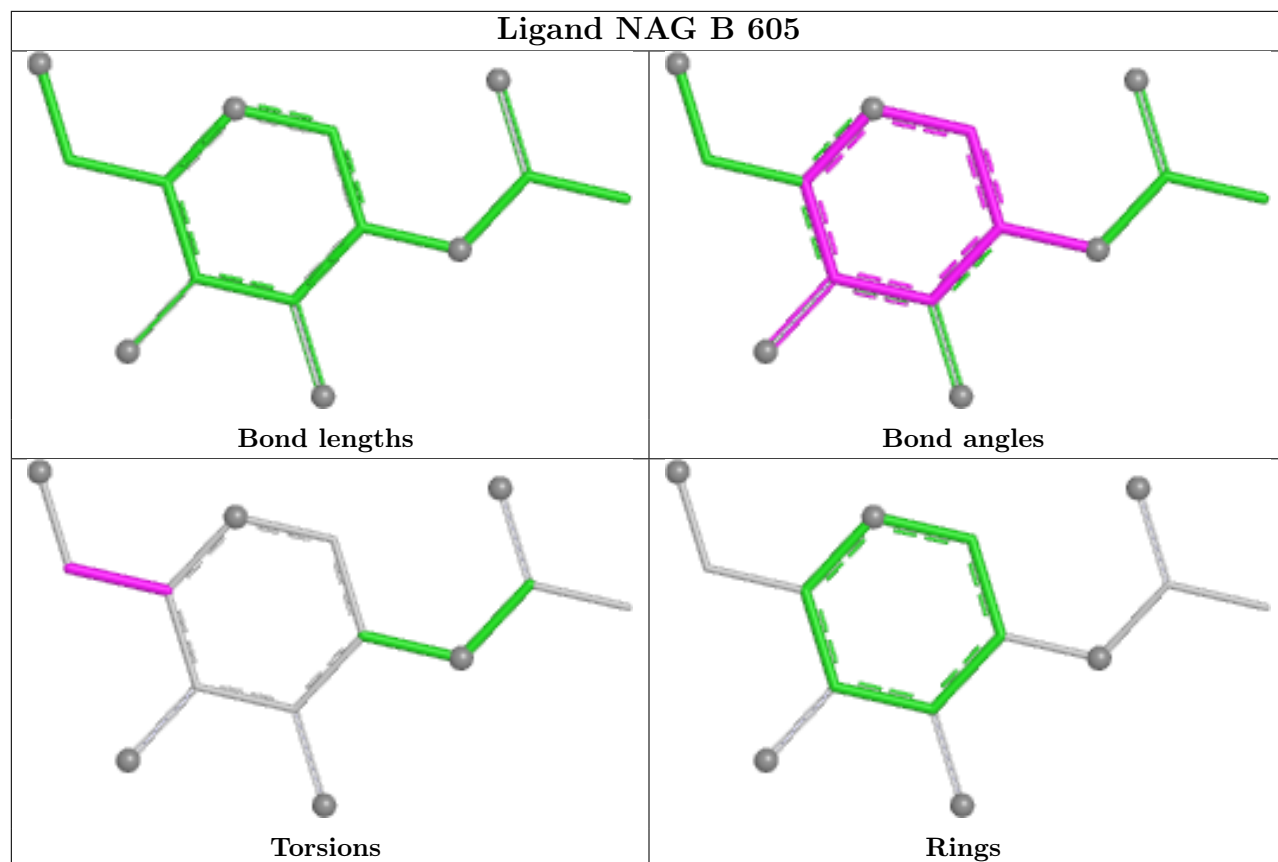
3 monomers are involved in 4 short contacts:

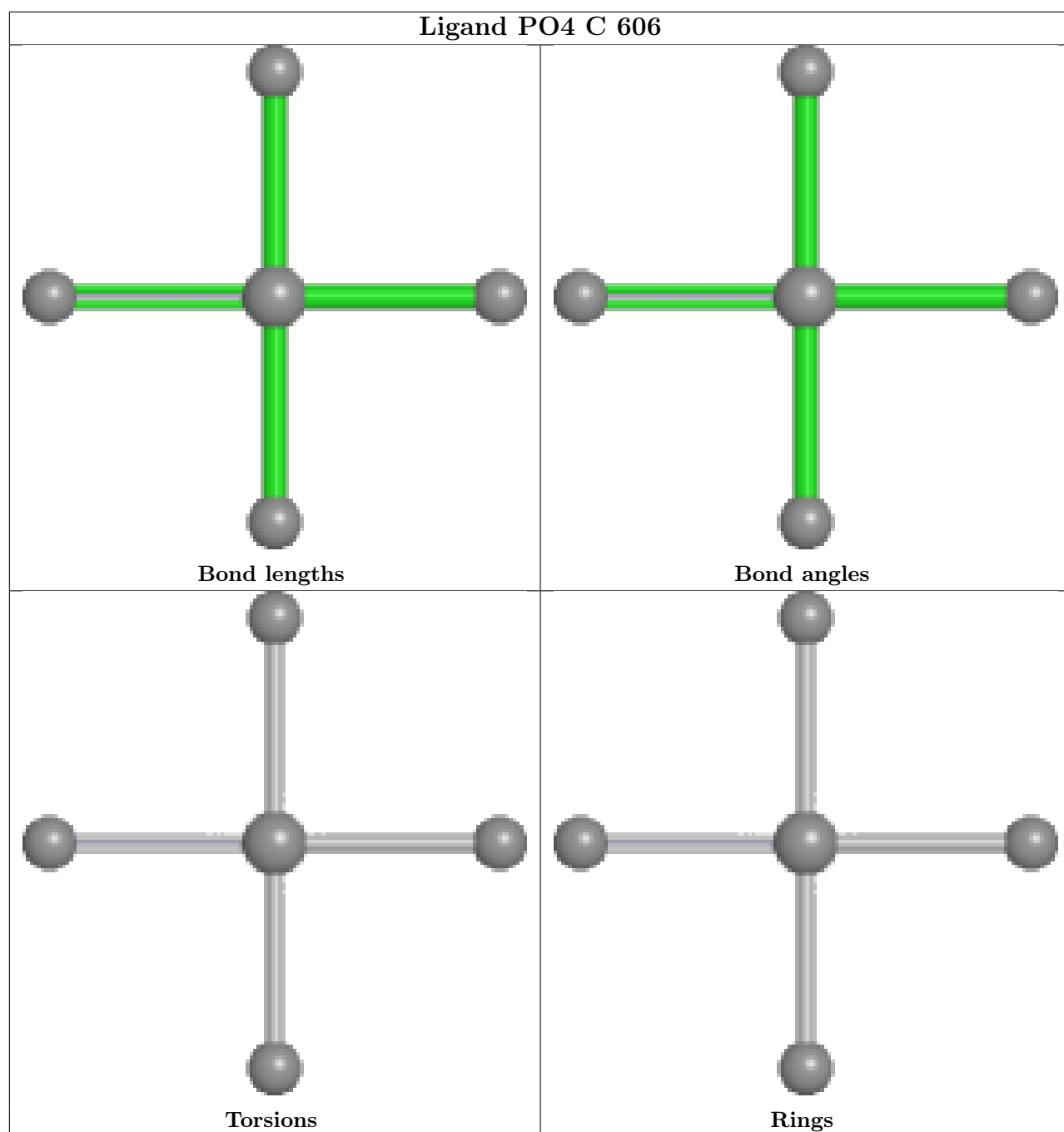
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	606	PO4	1	0
8	A	606	PO4	1	0
7	E	605	NAG	2	0

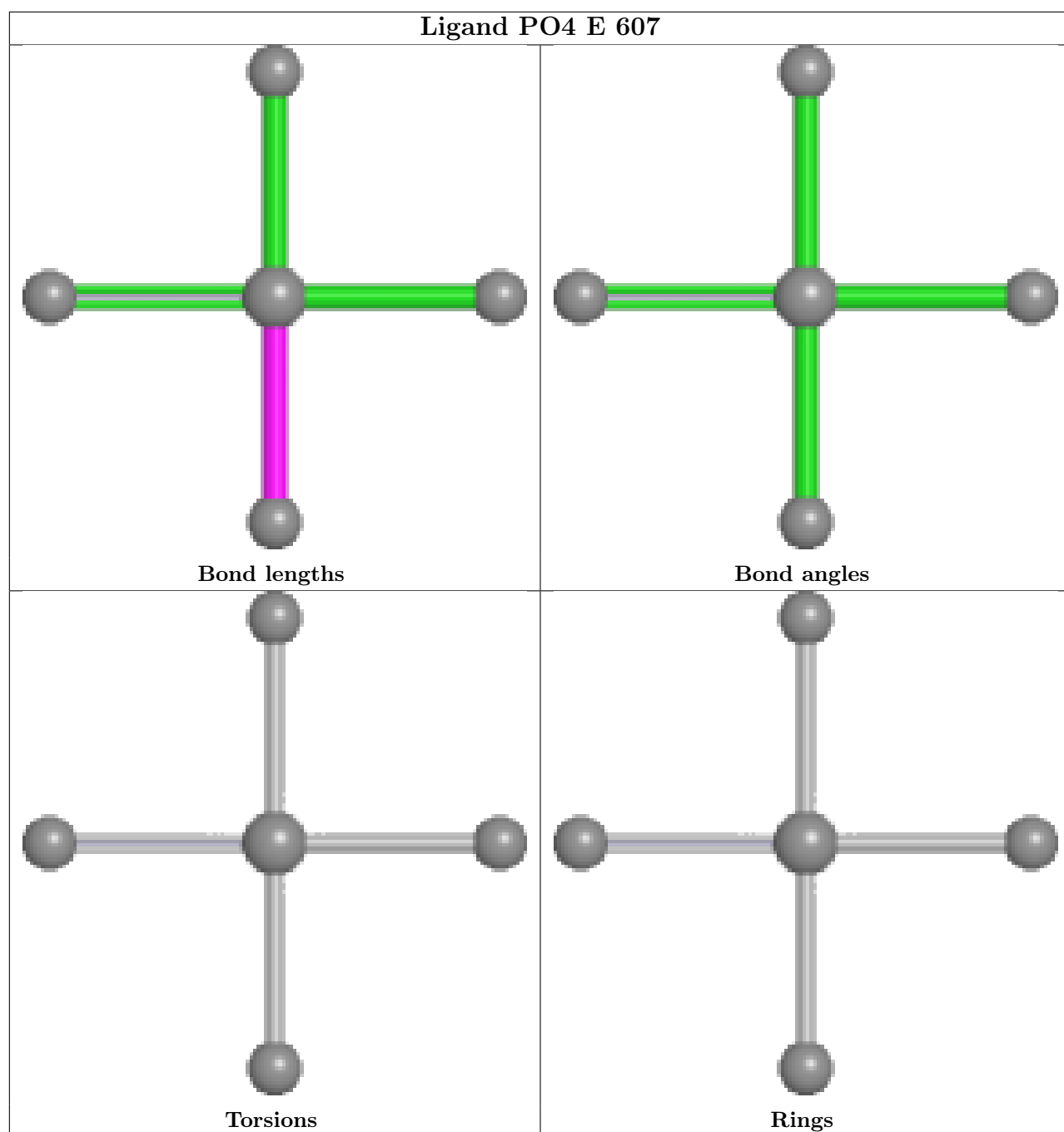
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

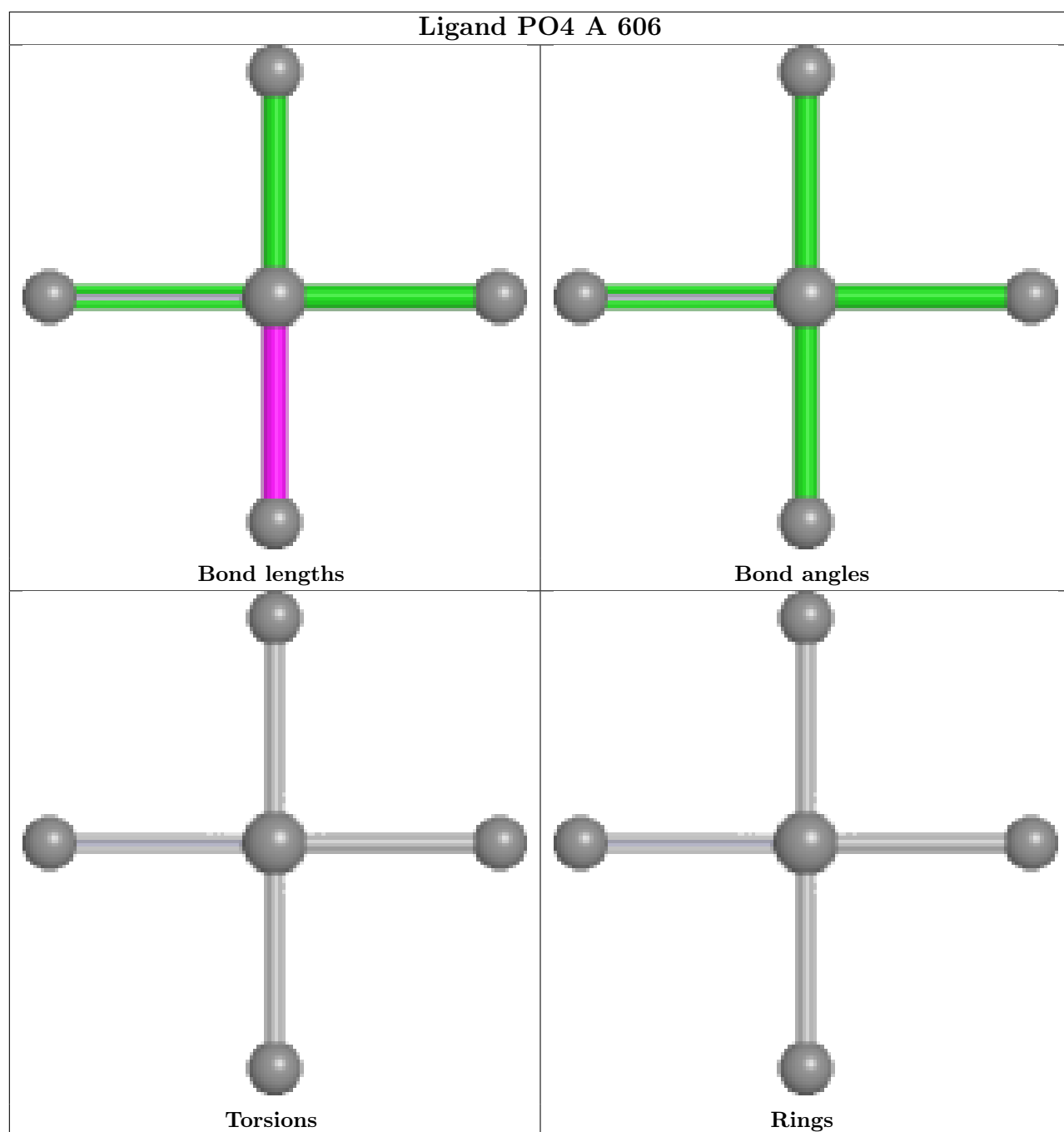


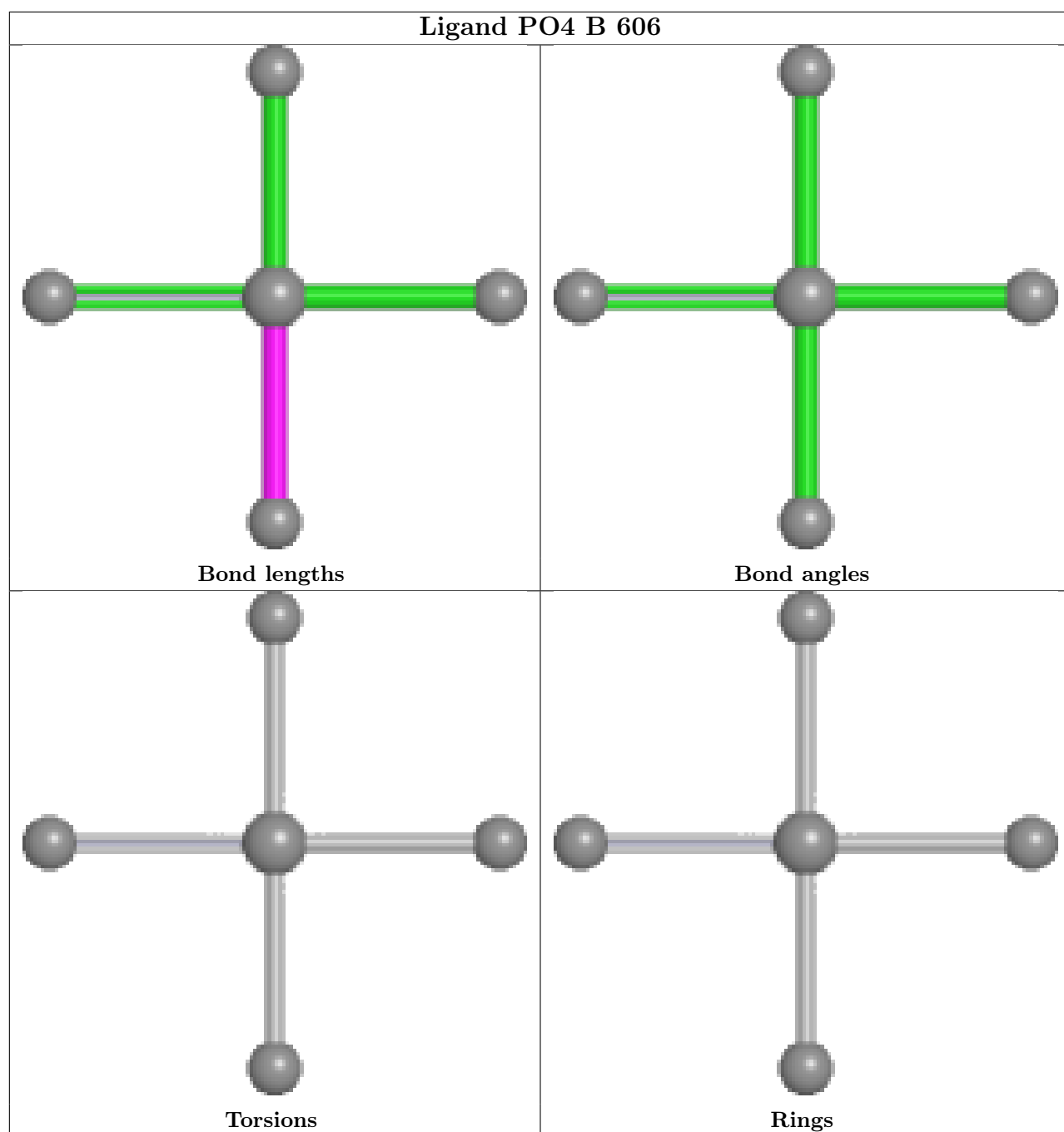


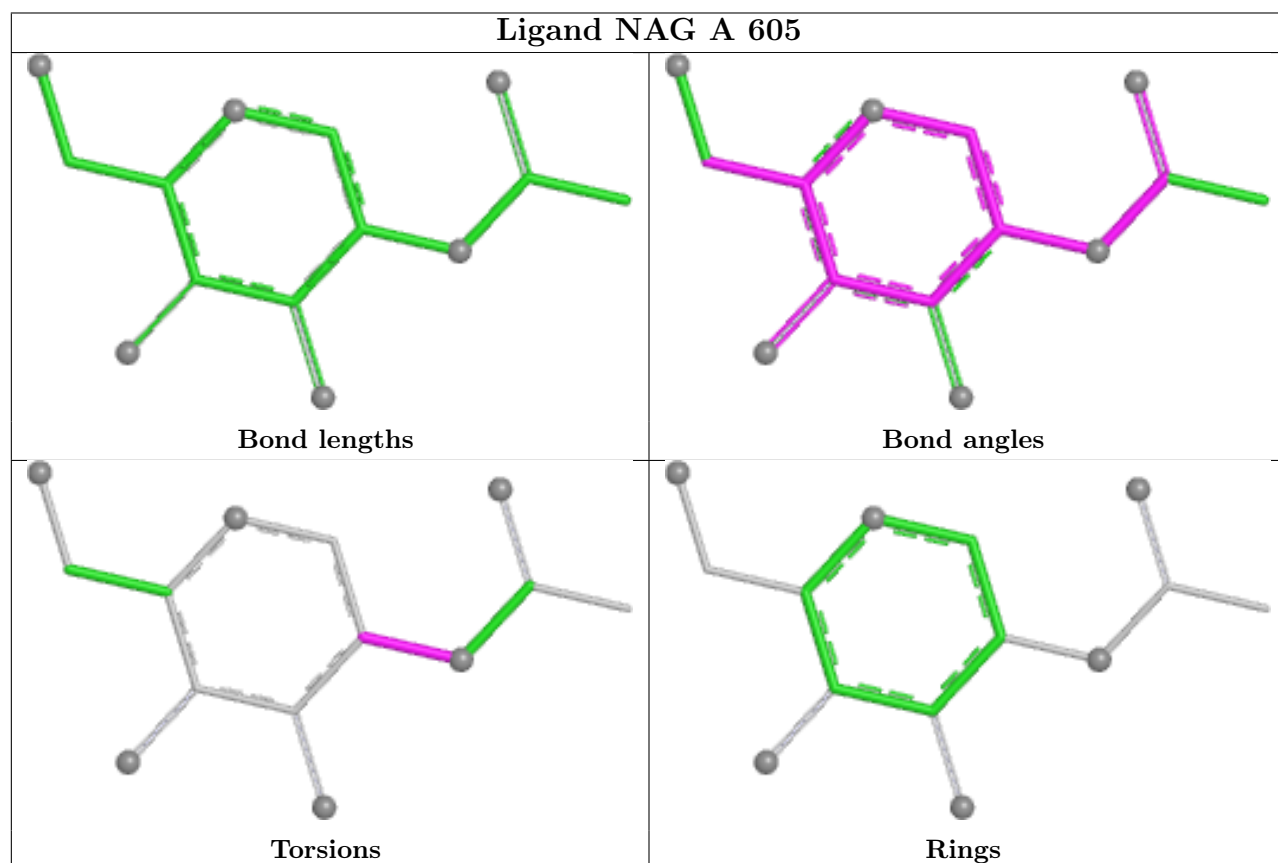
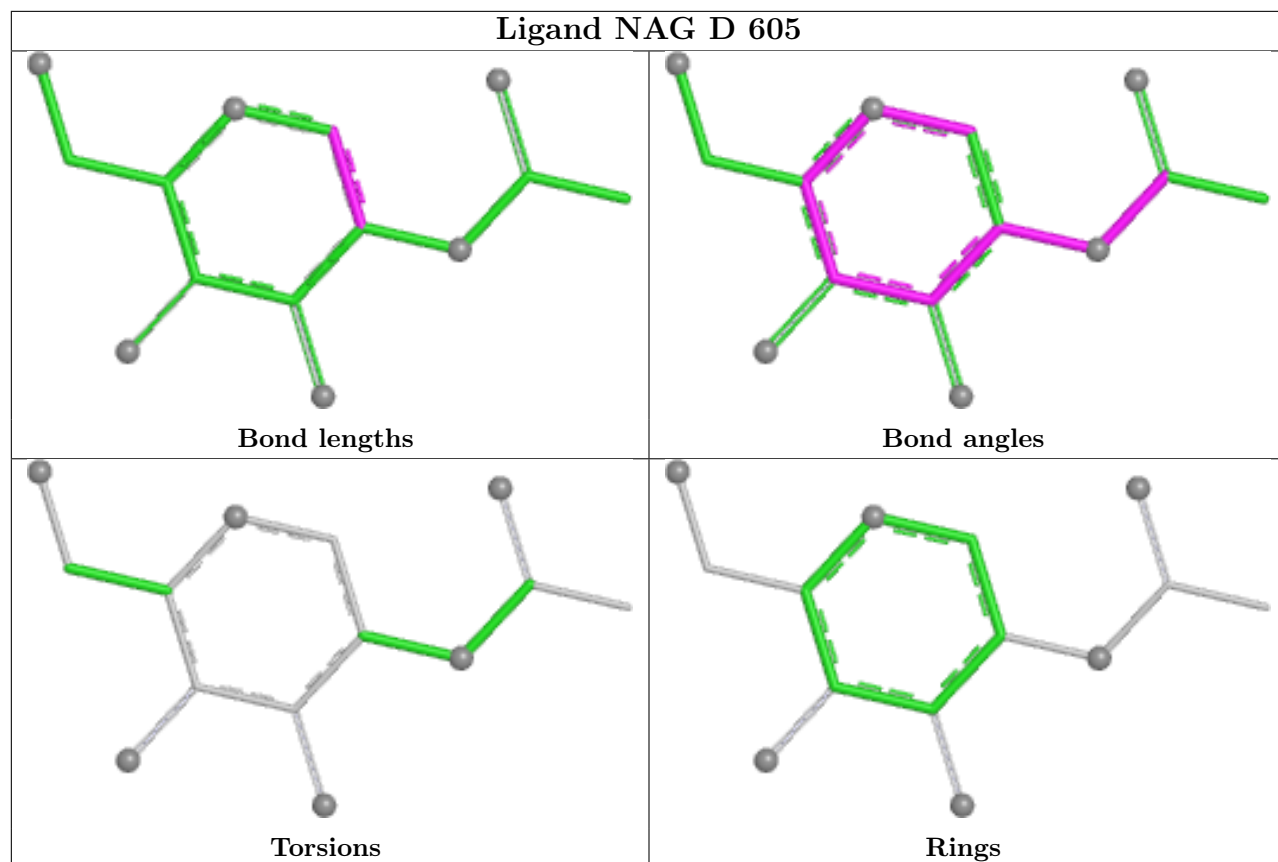


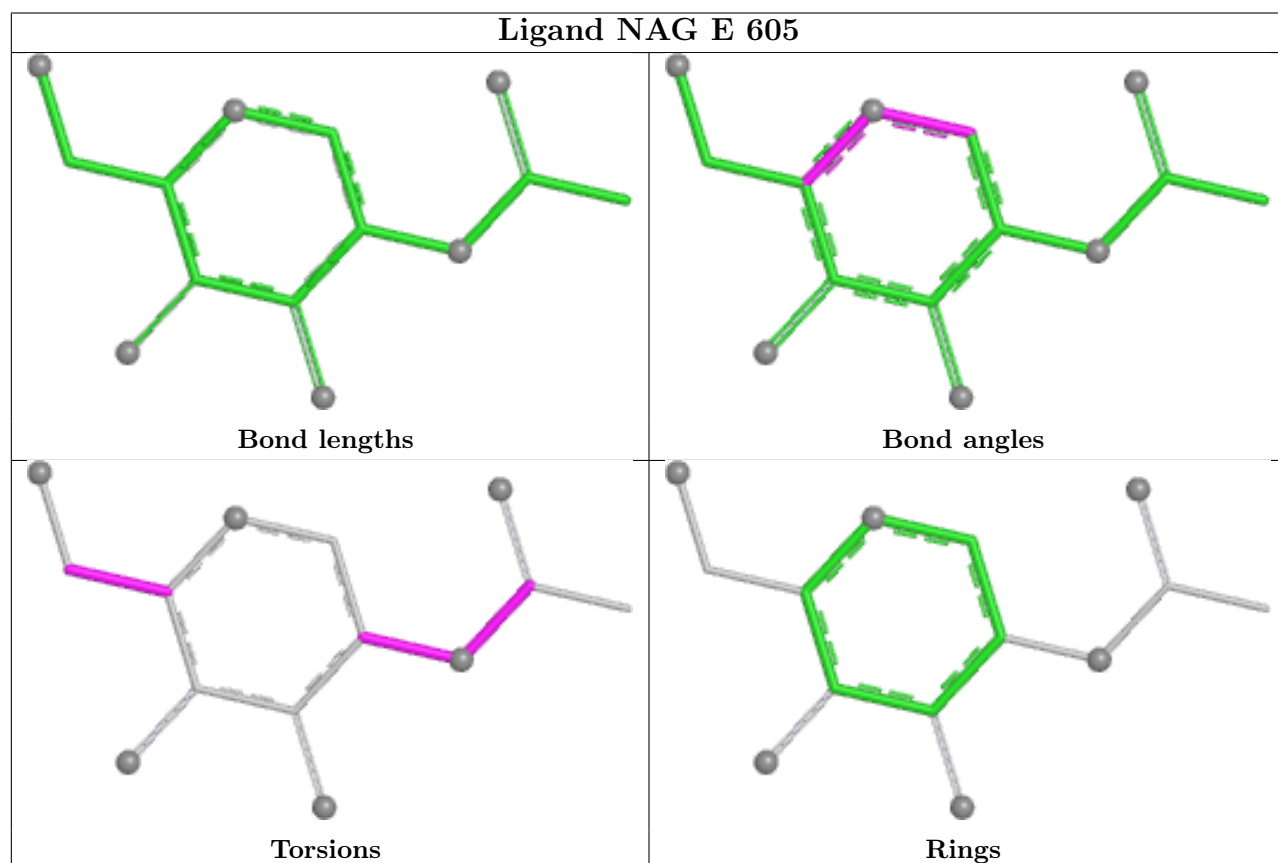
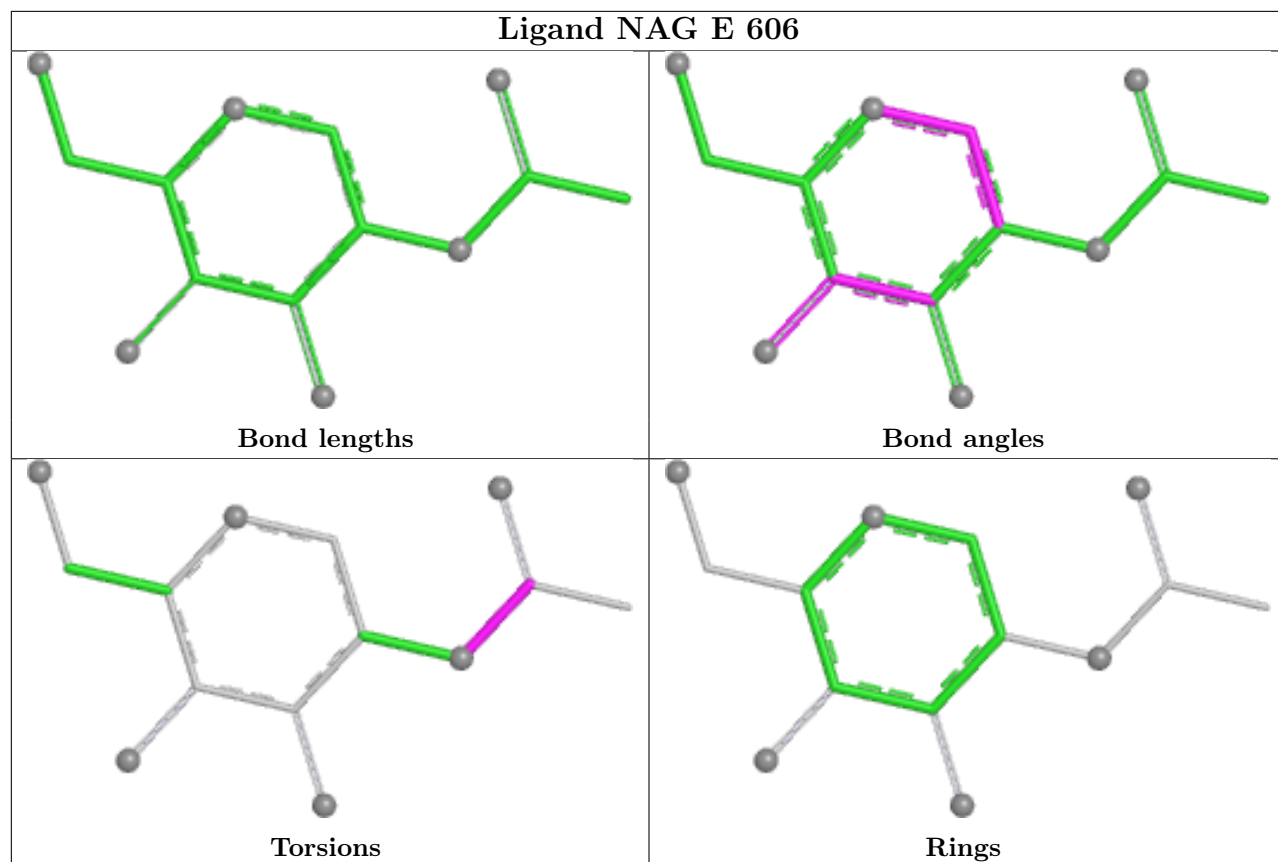












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	482/509 (94%)	0.13	4 (0%)	82 71	25, 60, 95, 137	0
1	B	482/509 (94%)	0.10	2 (0%)	88 81	30, 63, 101, 126	0
1	C	482/509 (94%)	0.16	4 (0%)	82 71	32, 68, 111, 138	0
1	D	483/509 (94%)	0.09	3 (0%)	85 75	34, 71, 112, 140	0
1	E	482/509 (94%)	0.21	6 (1%)	76 63	44, 83, 116, 142	0
All	All	2411/2545 (94%)	0.14	19 (0%)	82 71	25, 69, 109, 142	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	HIS	3.1
1	E	221	GLY	3.0
1	D	184	ARG	3.0
1	D	338	HIS	2.8
1	B	338	HIS	2.7
1	C	455	GLY	2.7
1	A	423	VAL	2.5
1	C	90	ASP	2.4
1	E	356	ASP	2.4
1	E	338	HIS	2.3
1	A	457	GLU	2.3
1	E	18	LEU	2.3
1	E	171	HIS	2.3
1	C	334	GLY	2.2
1	B	280	PRO	2.2
1	A	90	ASP	2.2
1	E	401	MET	2.1
1	D	104	ASN	2.1
1	C	409	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

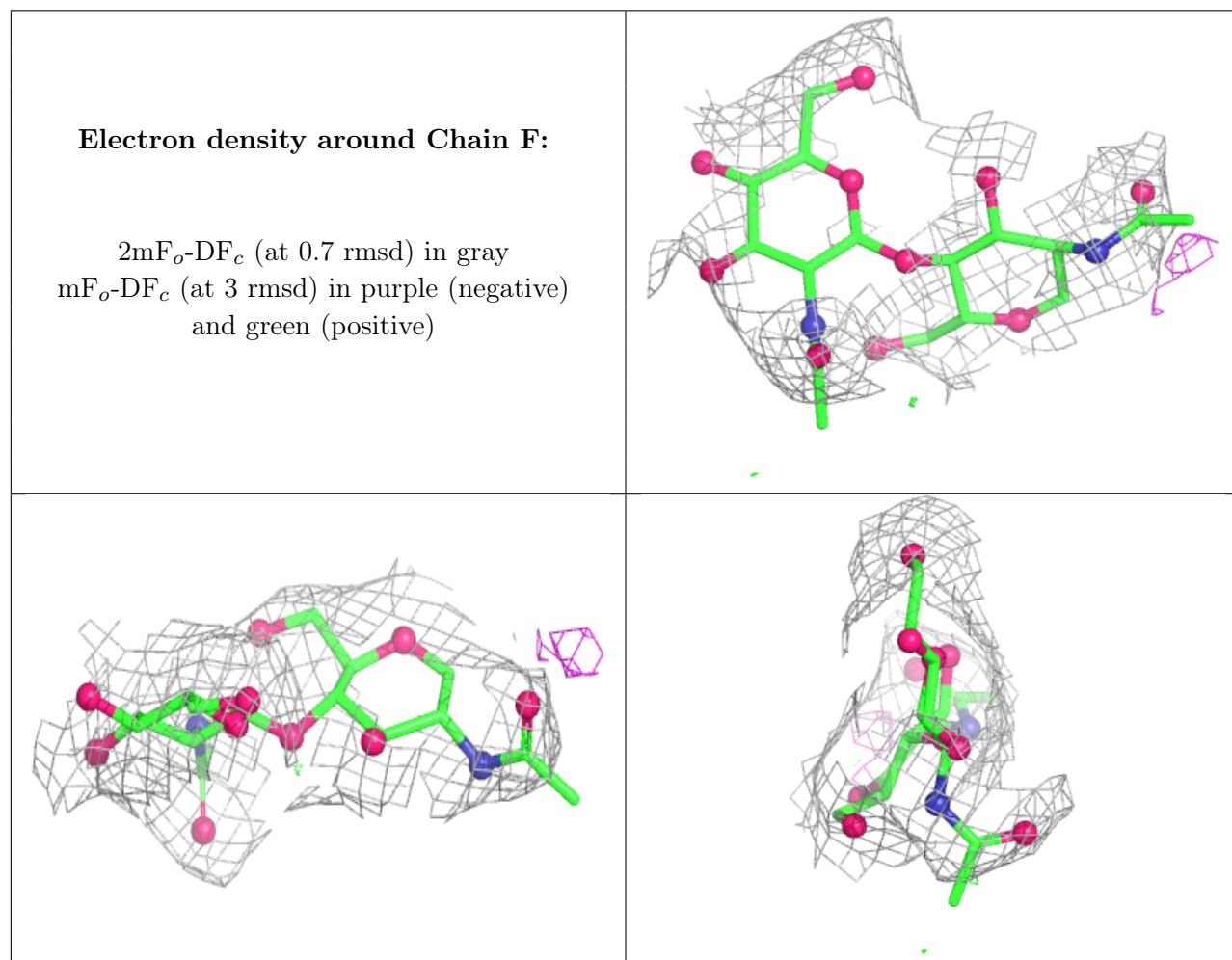
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

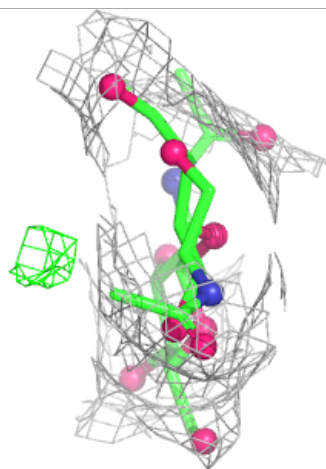
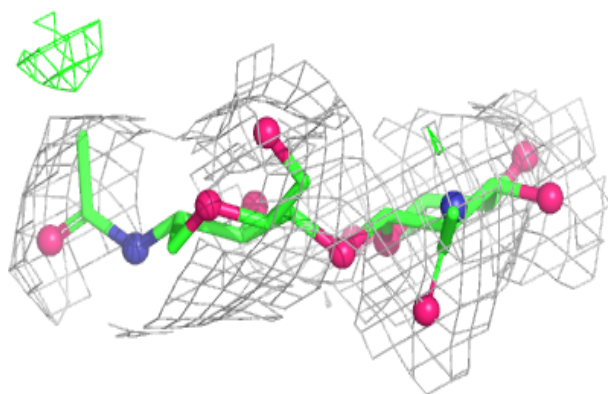
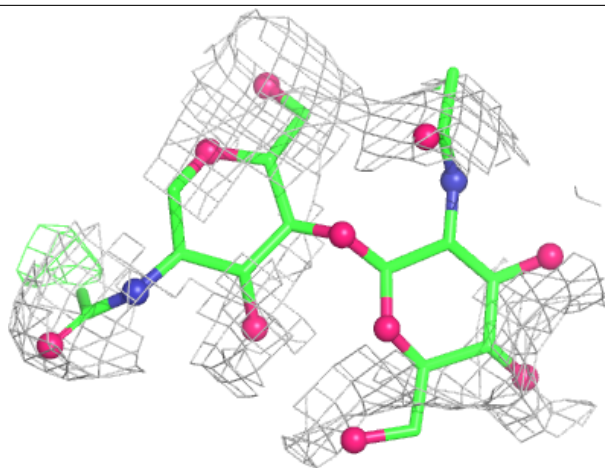
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	L	2	14/15	0.34	0.11	109,144,167,168	0
3	BMA	S	3	11/12	0.42	0.12	92,148,161,163	0
2	NAG	N	2	14/15	0.43	0.10	80,144,162,175	0
3	BMA	K	3	11/12	0.50	0.11	113,148,171,181	0
2	NAG	O	2	14/15	0.54	0.14	92,123,153,172	0
3	BMA	Q	3	11/12	0.55	0.14	100,162,172,184	0
2	NAG	R	2	14/15	0.60	0.12	125,142,157,174	0
3	BMA	H	3	11/12	0.61	0.15	125,149,156,169	0
2	NAG	L	1	14/15	0.63	0.10	100,151,161,161	0
3	NAG	S	2	14/15	0.68	0.11	85,122,161,165	0
2	NAG	I	2	14/15	0.69	0.10	61,115,138,139	0
2	NAG	M	2	14/15	0.69	0.11	100,129,146,148	0
2	NAG	J	2	14/15	0.70	0.12	110,122,135,142	0
2	NAG	P	2	14/15	0.70	0.11	94,128,152,153	0
2	NAG	F	2	14/15	0.72	0.09	94,123,137,160	0
2	NAG	G	2	14/15	0.73	0.11	106,131,137,142	0
2	NAG	M	1	14/15	0.76	0.11	92,105,119,123	0
3	NAG	K	2	14/15	0.76	0.10	88,118,145,161	0
3	NAG	H	2	14/15	0.76	0.09	117,136,160,169	0
2	NAG	R	1	14/15	0.77	0.12	100,133,151,152	0
2	NAG	G	1	14/15	0.78	0.10	70,94,128,131	0
3	NAG	S	1	14/15	0.78	0.09	67,114,127,128	0
3	NAG	K	1	14/15	0.82	0.10	66,101,118,119	0
3	NAG	Q	1	14/15	0.84	0.09	78,99,115,118	0
2	NAG	J	1	14/15	0.85	0.09	55,91,122,122	0
3	NAG	H	1	14/15	0.86	0.12	70,95,117,142	0
3	NAG	Q	2	14/15	0.86	0.09	125,142,168,169	0
2	NAG	P	1	14/15	0.86	0.09	68,93,118,124	0
2	NAG	N	1	14/15	0.88	0.07	65,82,113,124	0
2	NAG	O	1	14/15	0.91	0.09	78,94,108,138	0
2	NAG	I	1	14/15	0.91	0.09	81,101,118,129	0
2	NAG	F	1	14/15	0.92	0.09	85,99,125,134	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



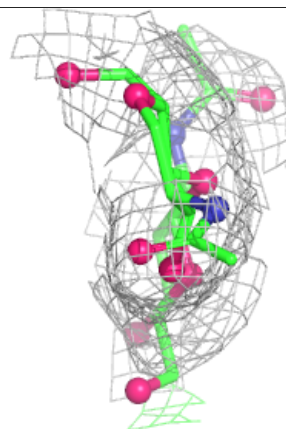
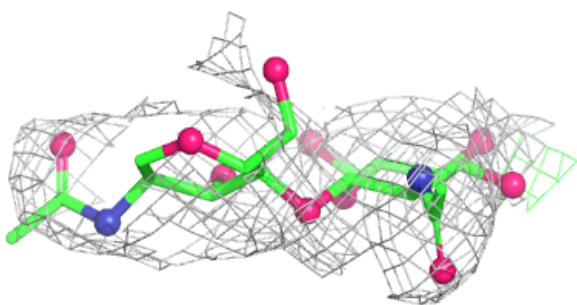
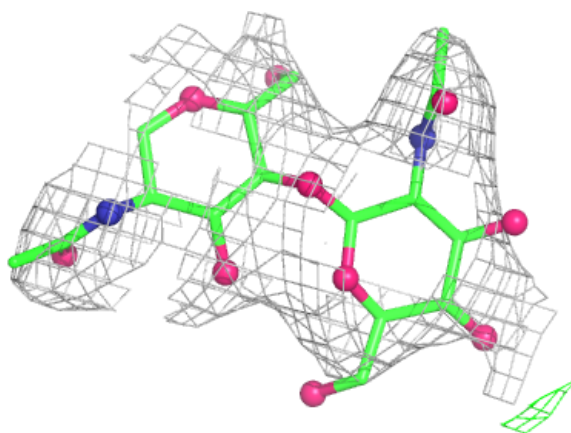
Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

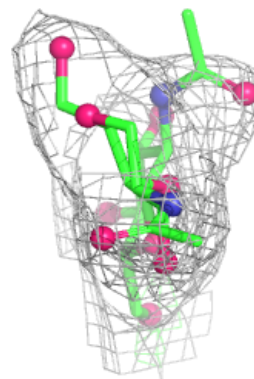
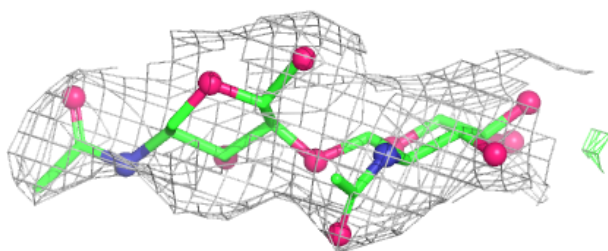
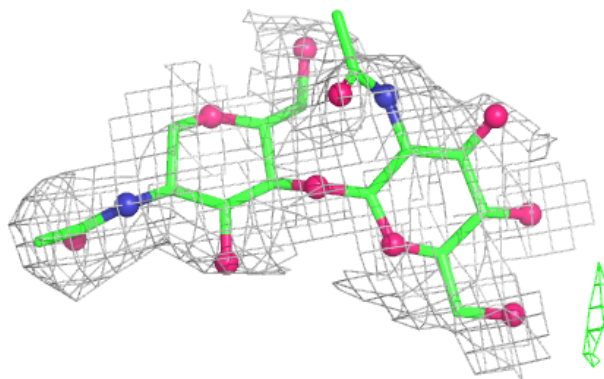


Electron density around Chain I:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

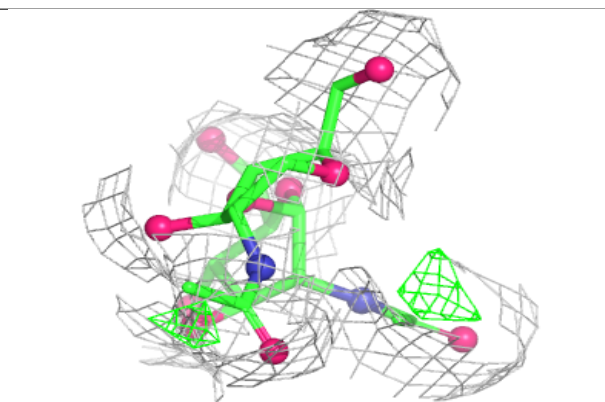
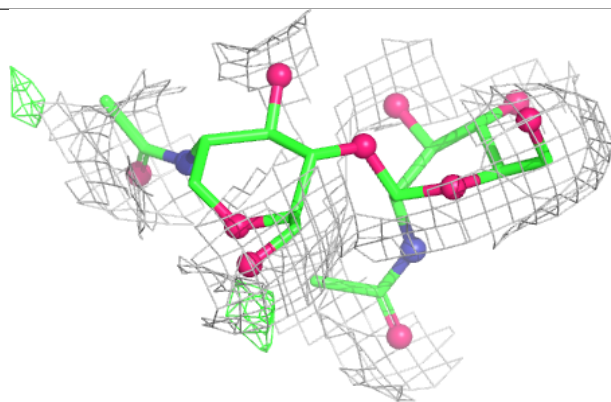
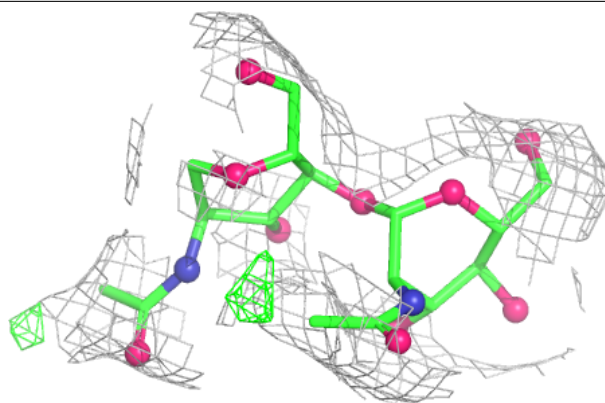
**Electron density around Chain J:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

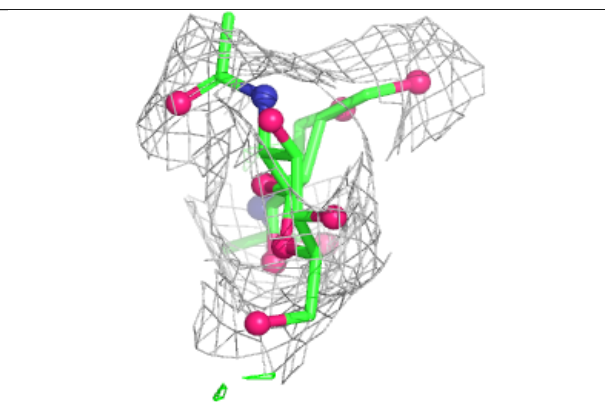
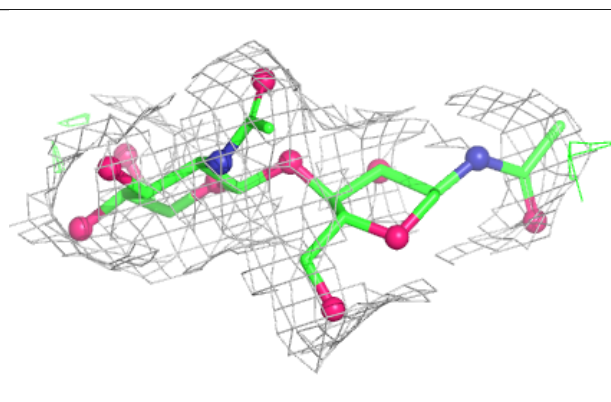
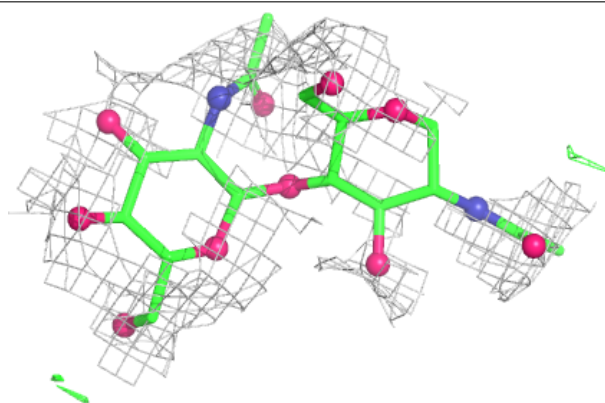


Electron density around Chain L:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

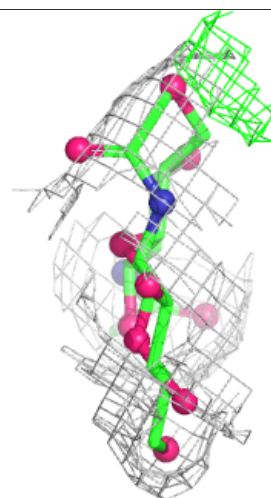
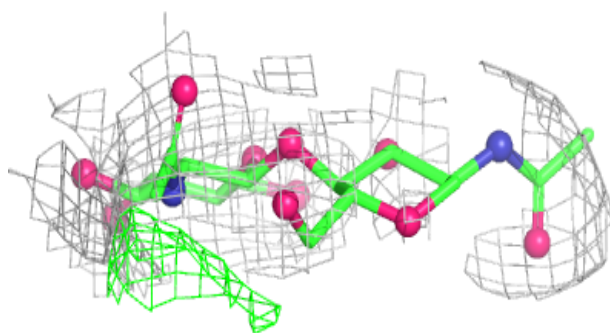
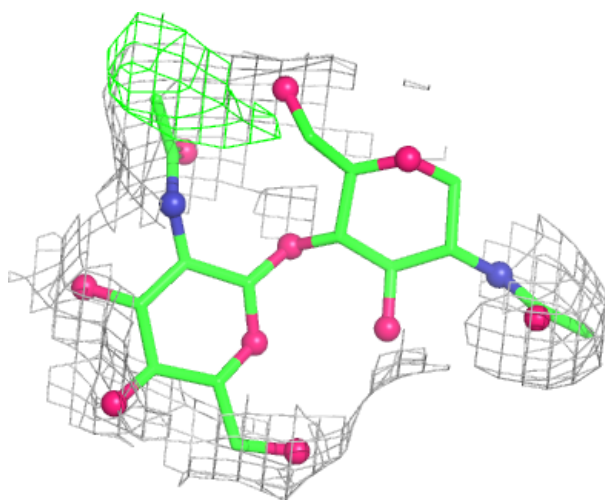
**Electron density around Chain M:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



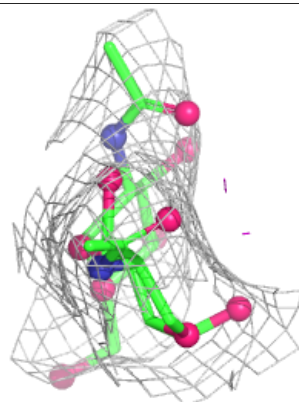
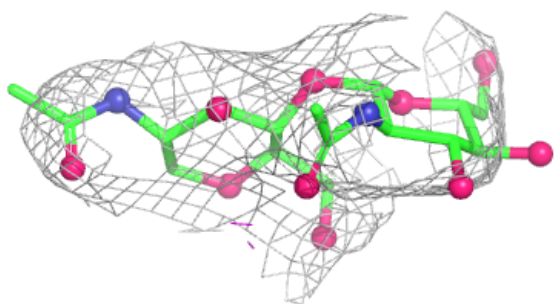
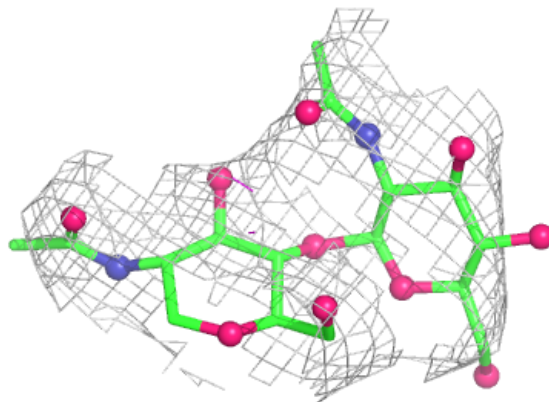
Electron density around Chain N:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

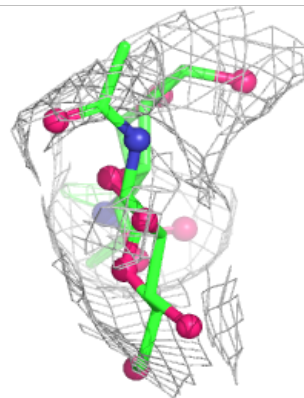
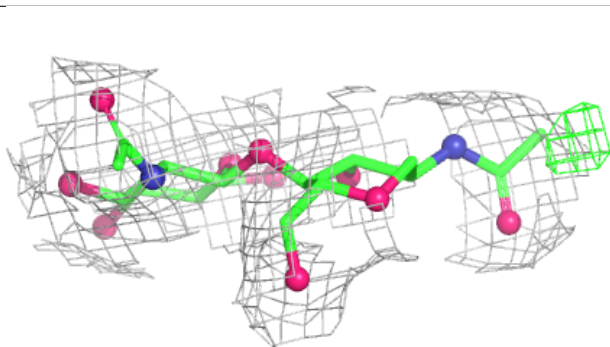
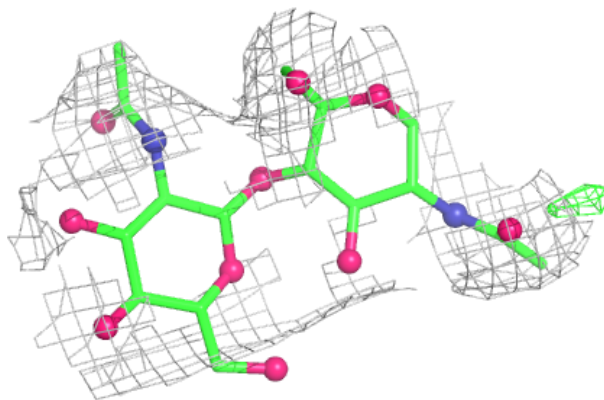


Electron density around Chain O:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

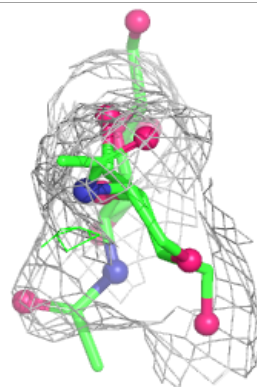
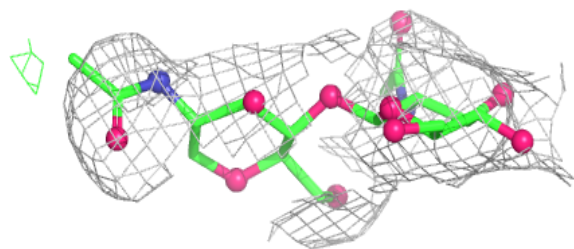
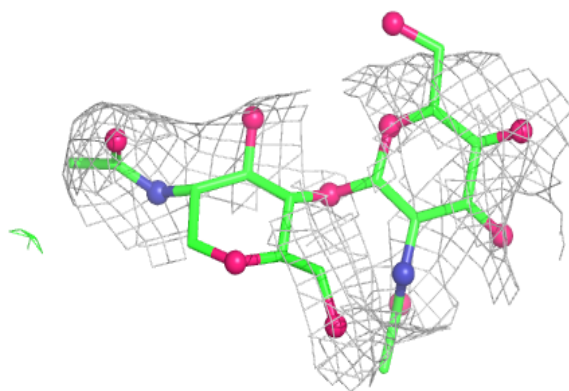
**Electron density around Chain P:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

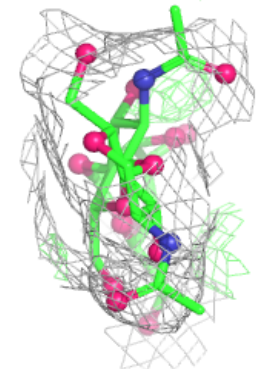
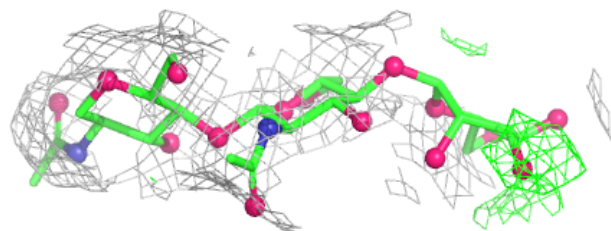
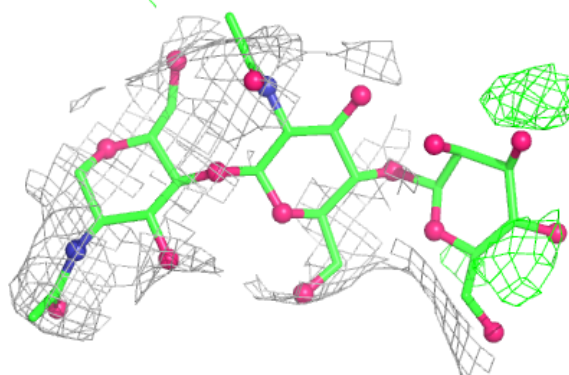


Electron density around Chain R:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

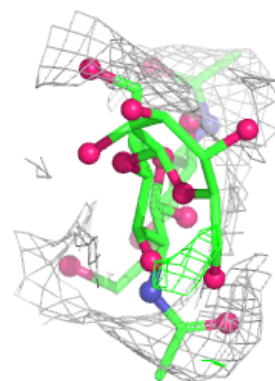
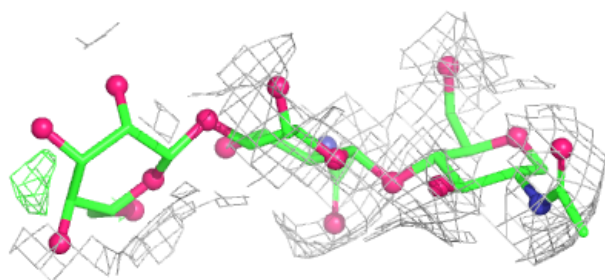
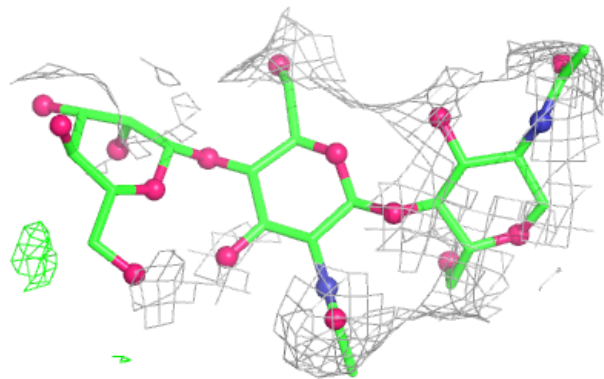
**Electron density around Chain H:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

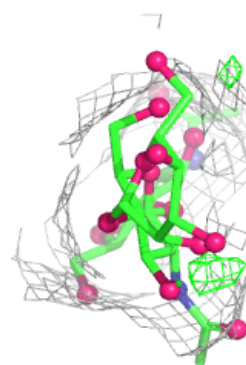
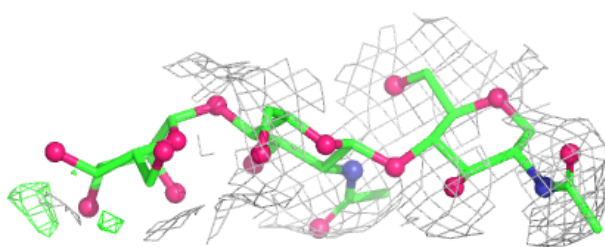
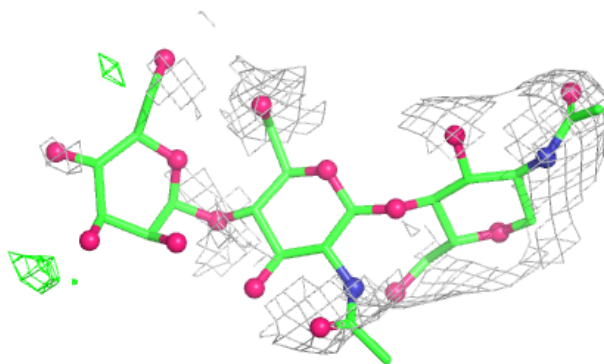


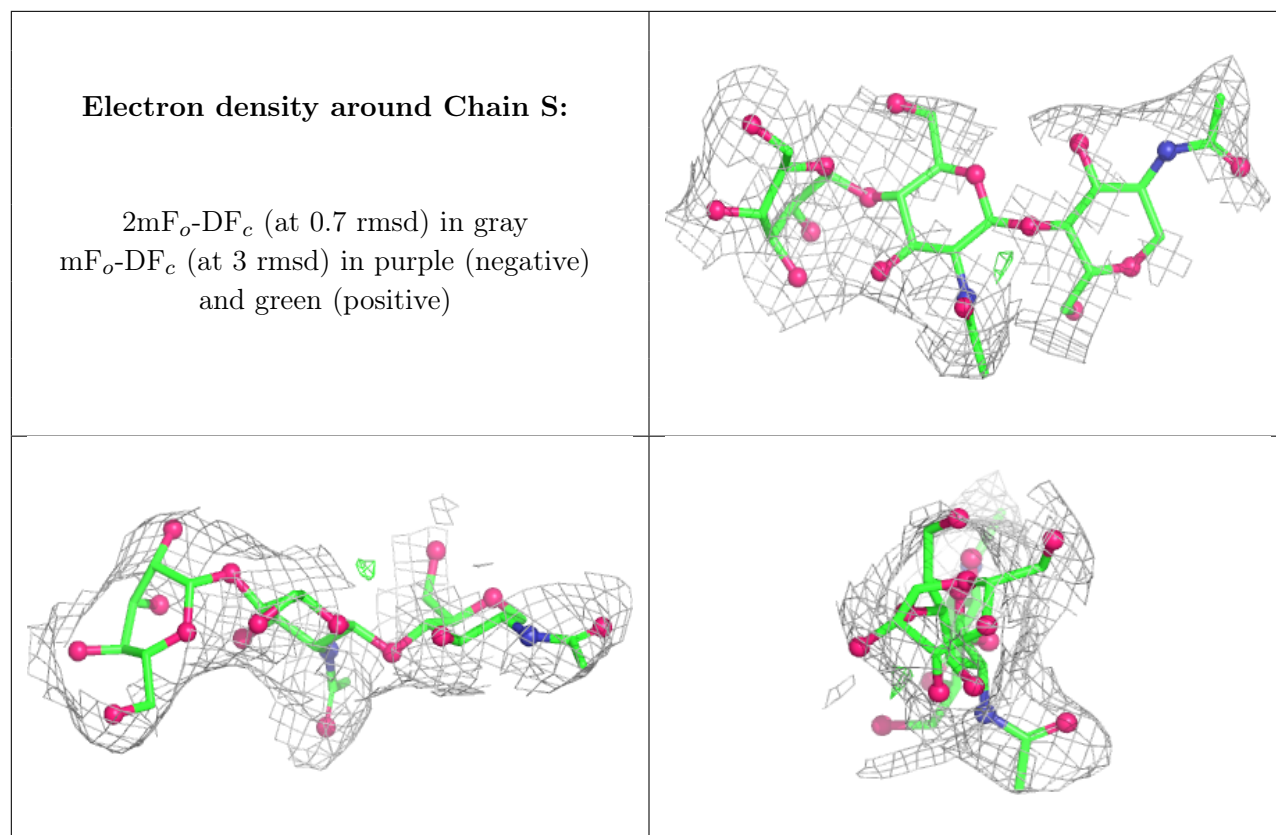
Electron density around Chain K:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain Q:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	D	605	14/15	0.51	0.15	105,172,188,191	0
7	NAG	E	605	14/15	0.52	0.18	70,122,138,155	0
7	NAG	A	605	14/15	0.56	0.15	73,123,132,142	0
7	NAG	E	606	14/15	0.61	0.12	82,109,142,144	0
7	NAG	B	605	14/15	0.79	0.10	81,128,157,159	0
8	PO4	D	606	5/5	0.82	0.16	115,116,154,161	0
5	MG	C	603	1/1	0.84	0.17	62,62,62,62	0
8	PO4	A	606	5/5	0.87	0.13	91,97,118,124	0
7	NAG	C	605	14/15	0.87	0.11	70,98,117,150	0
8	PO4	B	606	5/5	0.90	0.14	76,86,114,126	0
5	MG	E	603	1/1	0.90	0.16	95,95,95,95	0
8	PO4	C	606	5/5	0.91	0.14	82,100,116,119	0
4	ZN	E	602	1/1	0.91	0.09	207,207,207,207	0
5	MG	B	603	1/1	0.92	0.19	67,67,67,67	0

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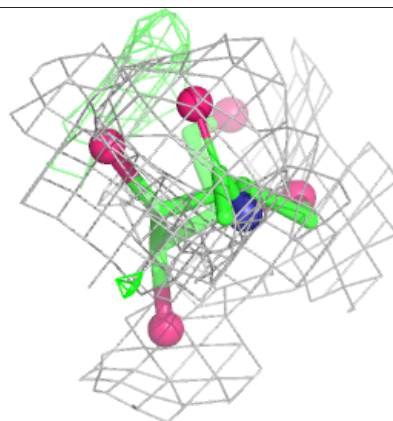
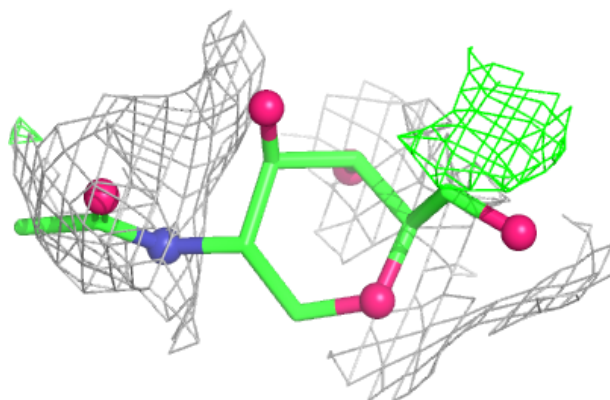
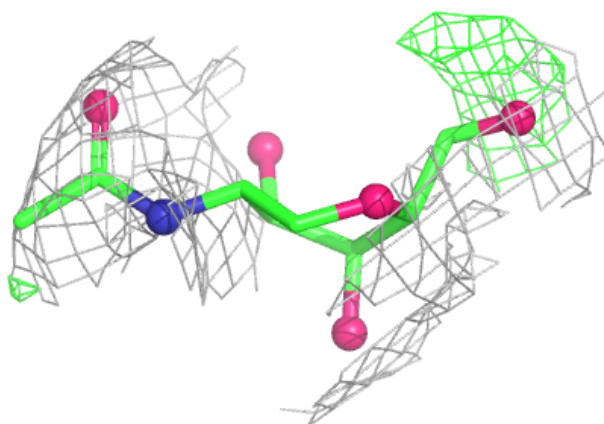
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	E	604	1/1	0.94	0.09	116,116,116,116	0
8	PO4	E	607	5/5	0.94	0.09	92,116,130,141	0
5	MG	A	603	1/1	0.95	0.11	35,35,35,35	0
5	MG	D	603	1/1	0.95	0.11	60,60,60,60	0
4	ZN	D	602	1/1	0.95	0.06	195,195,195,195	0
4	ZN	B	602	1/1	0.96	0.09	228,228,228,228	0
4	ZN	C	601	1/1	0.97	0.12	193,193,193,193	0
4	ZN	C	602	1/1	0.97	0.05	151,151,151,151	0
6	CA	A	604	1/1	0.97	0.11	83,83,83,83	0
4	ZN	B	601	1/1	0.97	0.10	94,94,94,94	0
4	ZN	E	601	1/1	0.97	0.05	80,80,80,80	0
6	CA	B	604	1/1	0.98	0.04	92,92,92,92	0
6	CA	C	604	1/1	0.98	0.03	90,90,90,90	0
6	CA	D	604	1/1	0.98	0.05	93,93,93,93	0
4	ZN	D	601	1/1	0.98	0.03	84,84,84,84	0
4	ZN	A	602	1/1	0.98	0.05	160,160,160,160	0
4	ZN	A	601	1/1	0.99	0.03	56,56,56,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

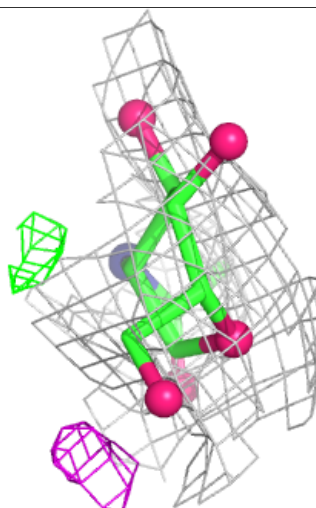
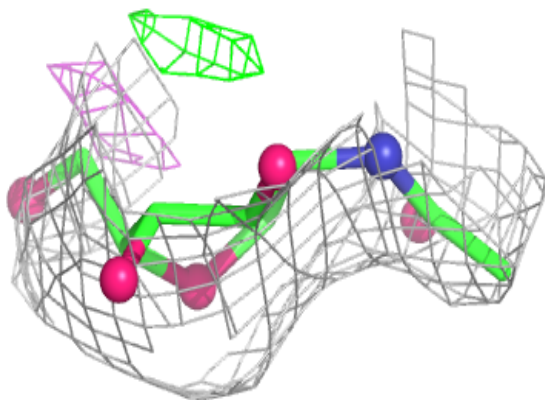
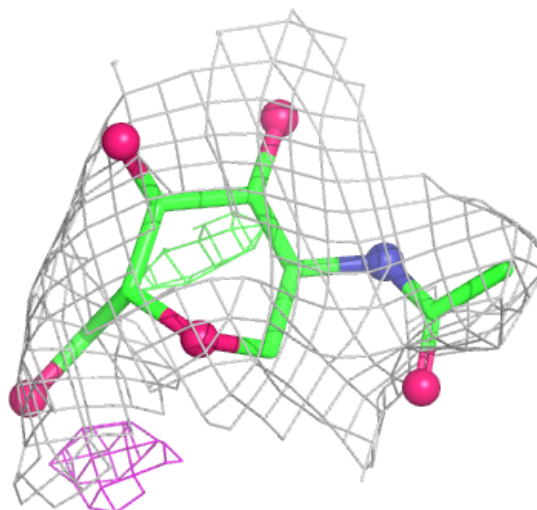
Electron density around NAG D 605:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



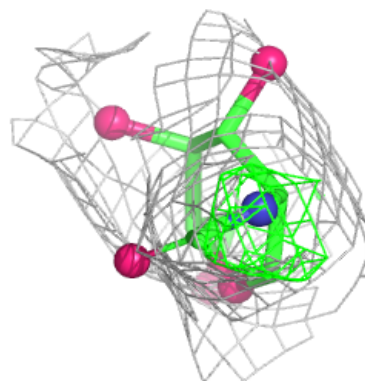
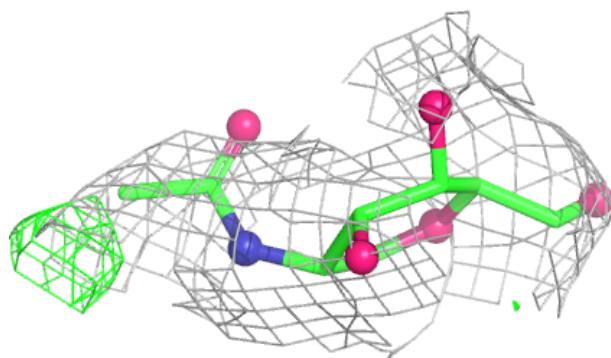
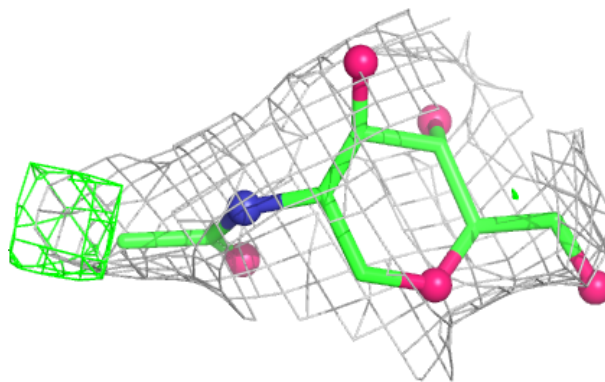
Electron density around NAG E 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



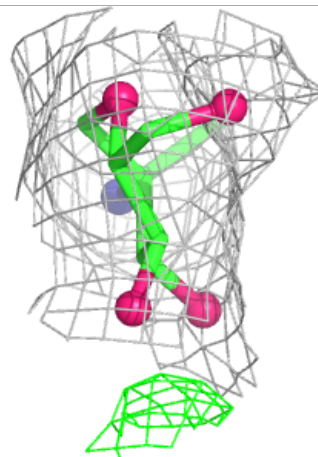
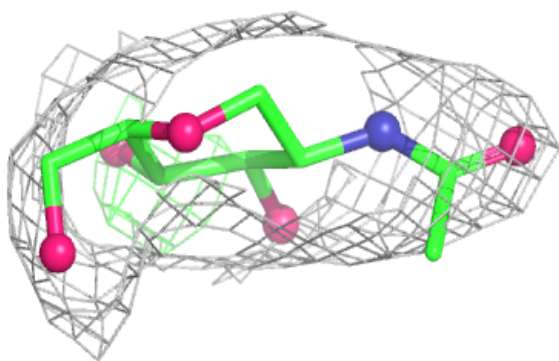
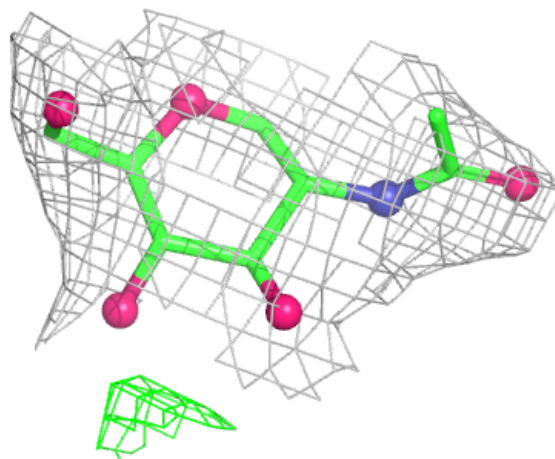
Electron density around NAG A 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



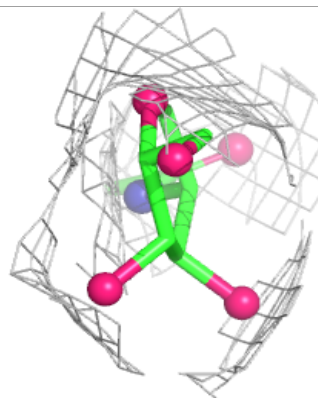
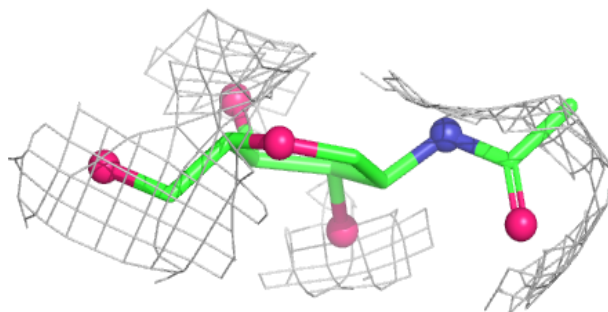
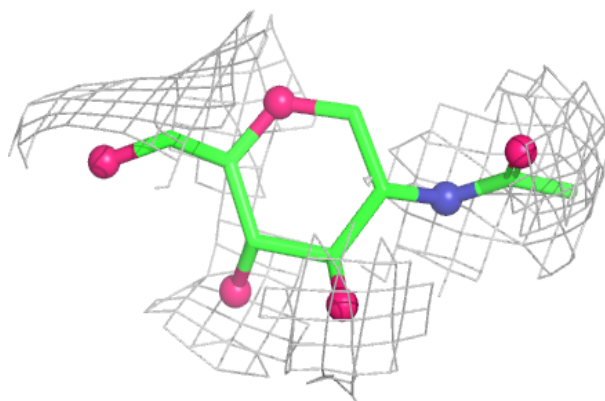
Electron density around NAG E 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



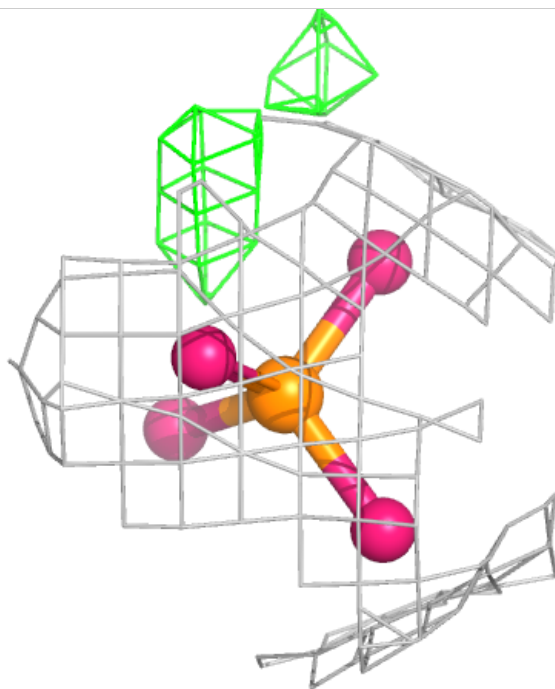
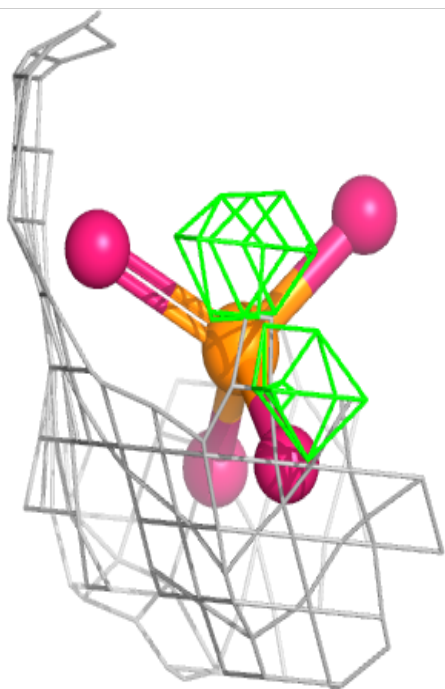
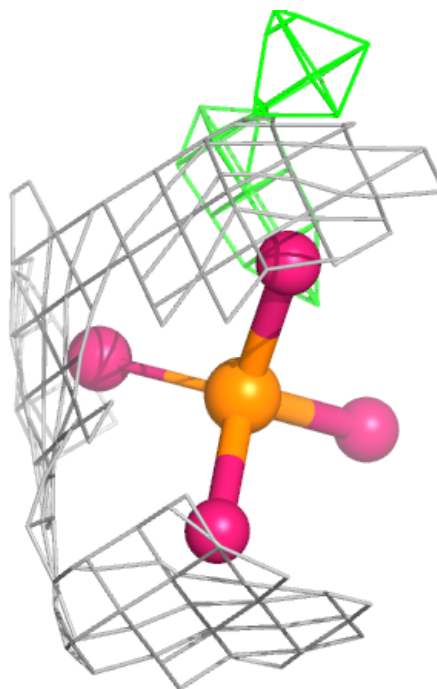
Electron density around NAG B 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



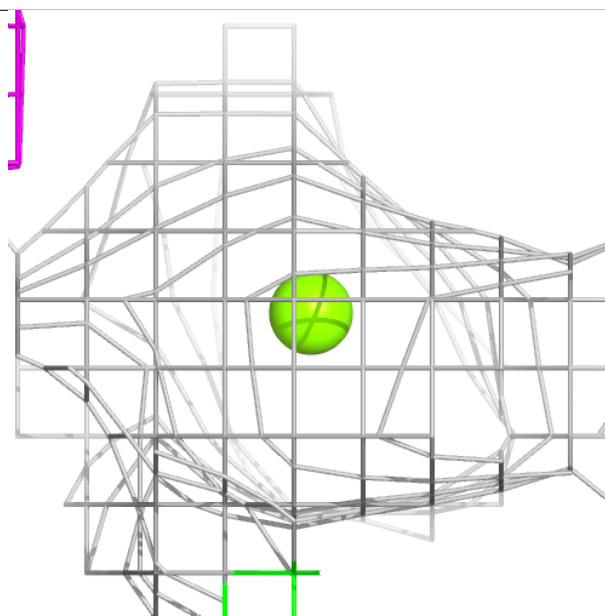
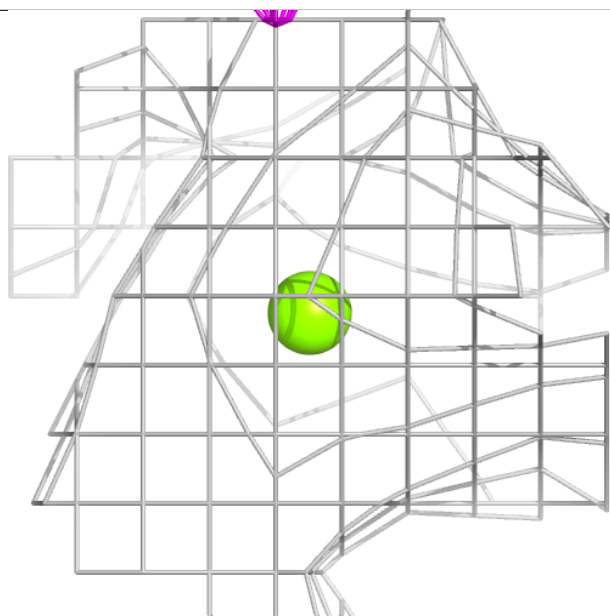
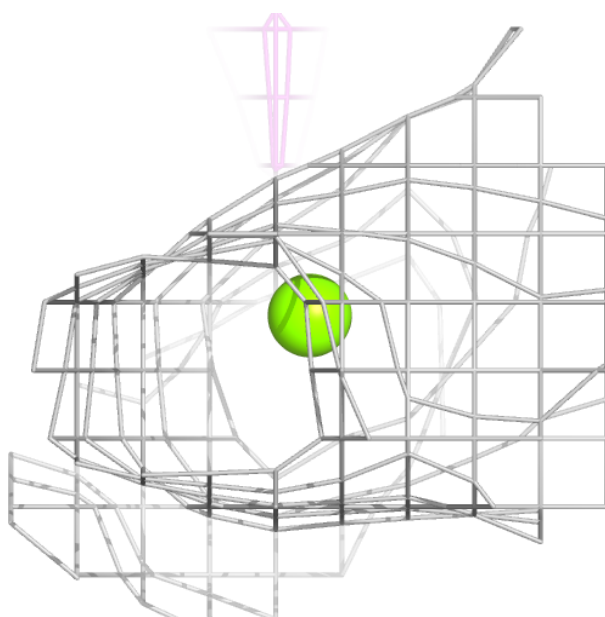
Electron density around PO4 D 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



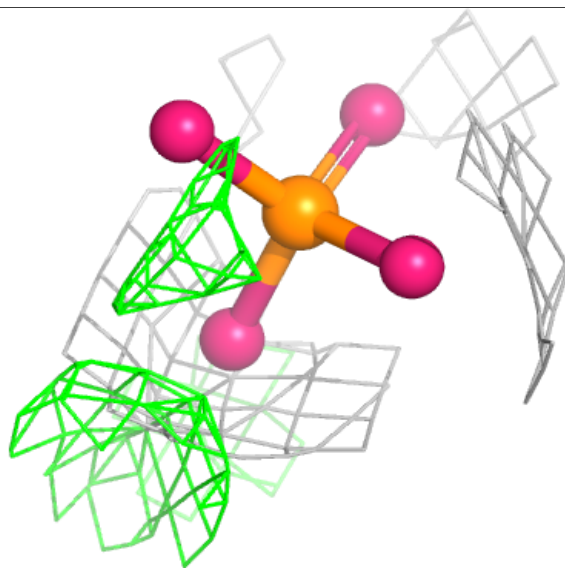
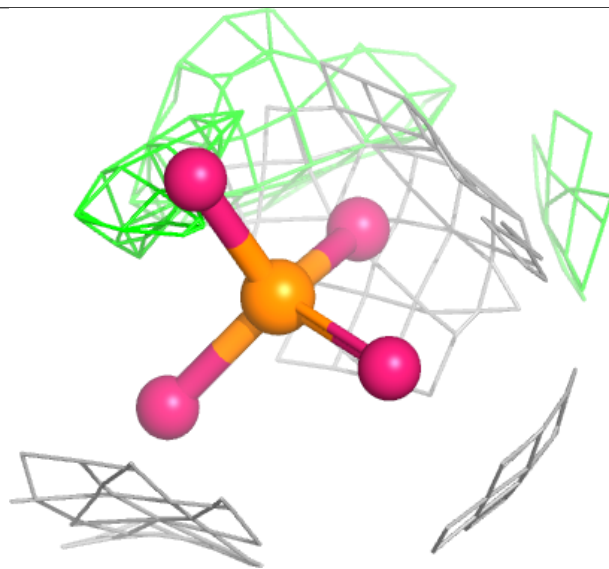
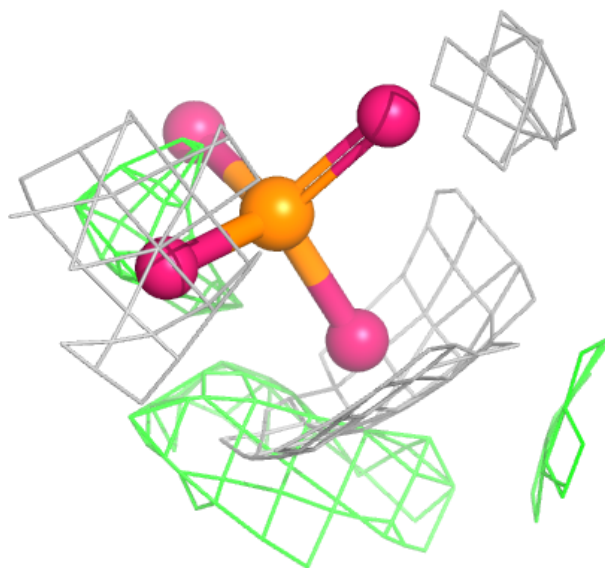
Electron density around MG C 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



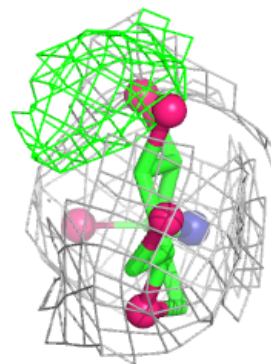
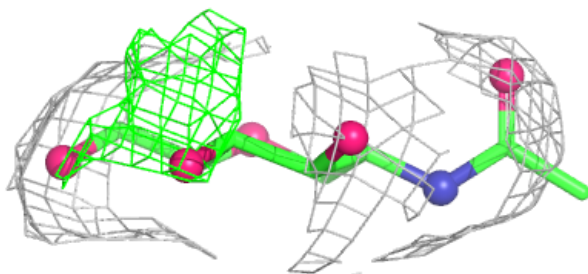
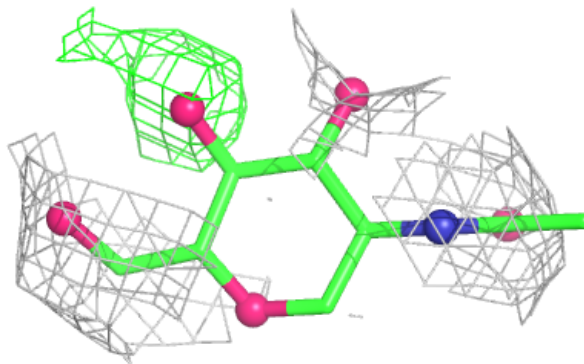
Electron density around PO4 A 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



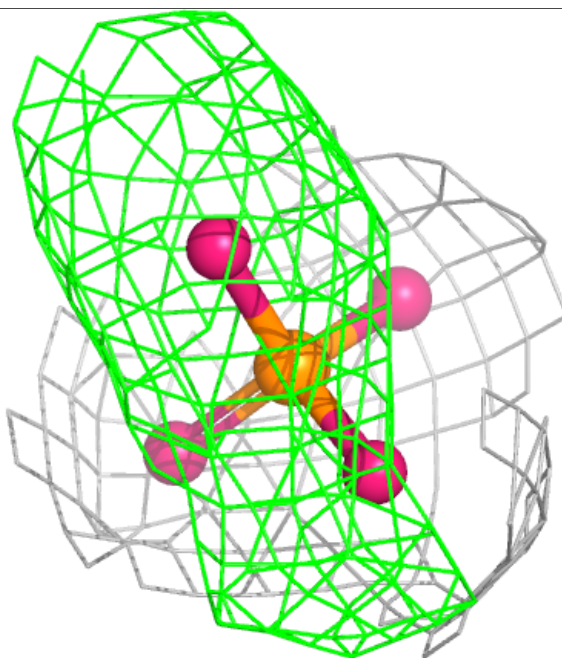
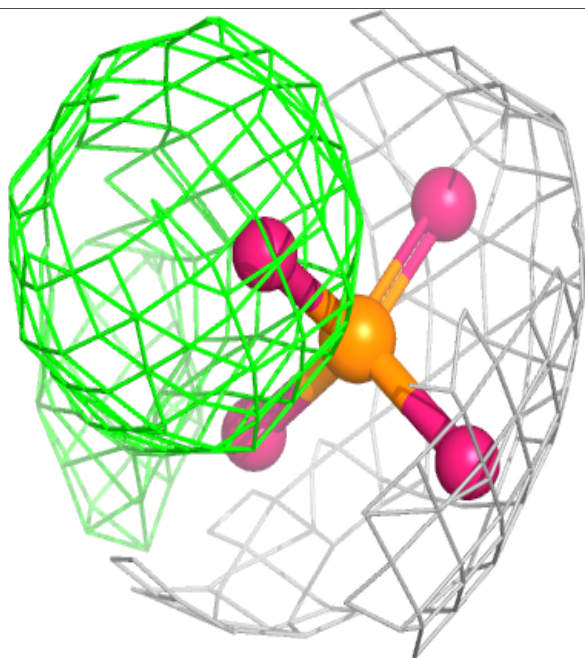
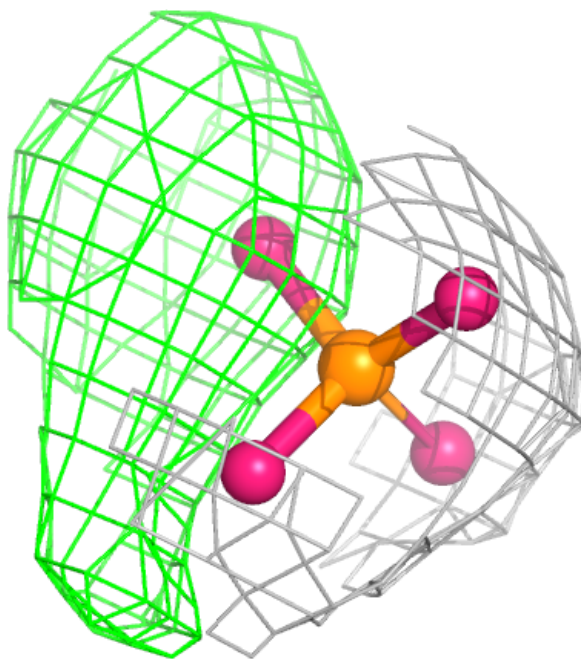
Electron density around NAG C 605:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



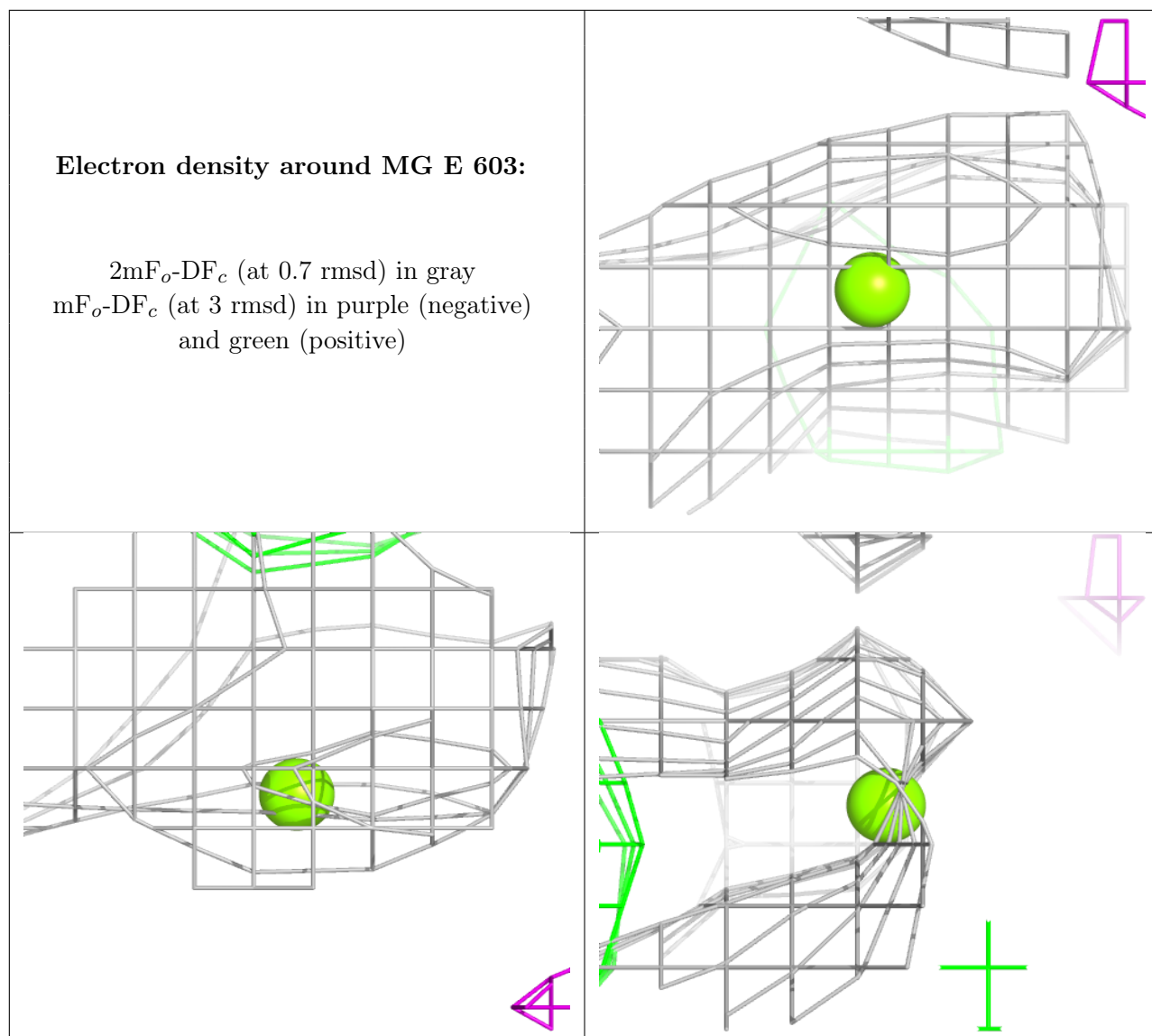
Electron density around PO4 B 606:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



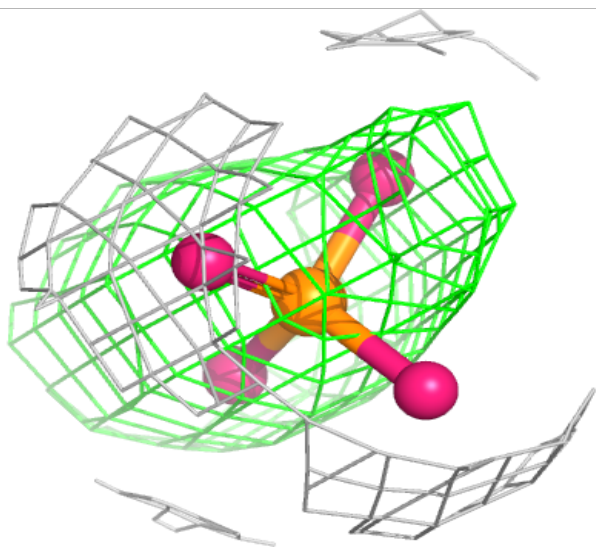
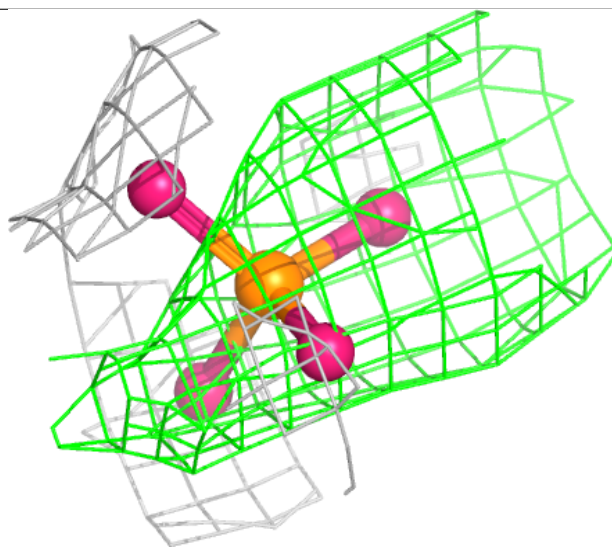
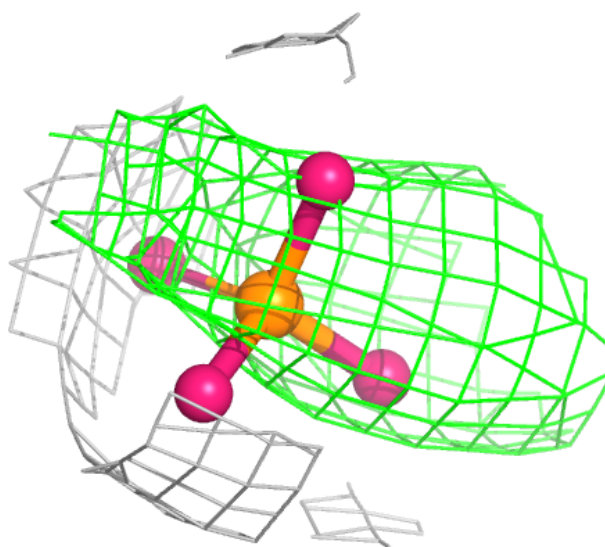
Electron density around MG E 603:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



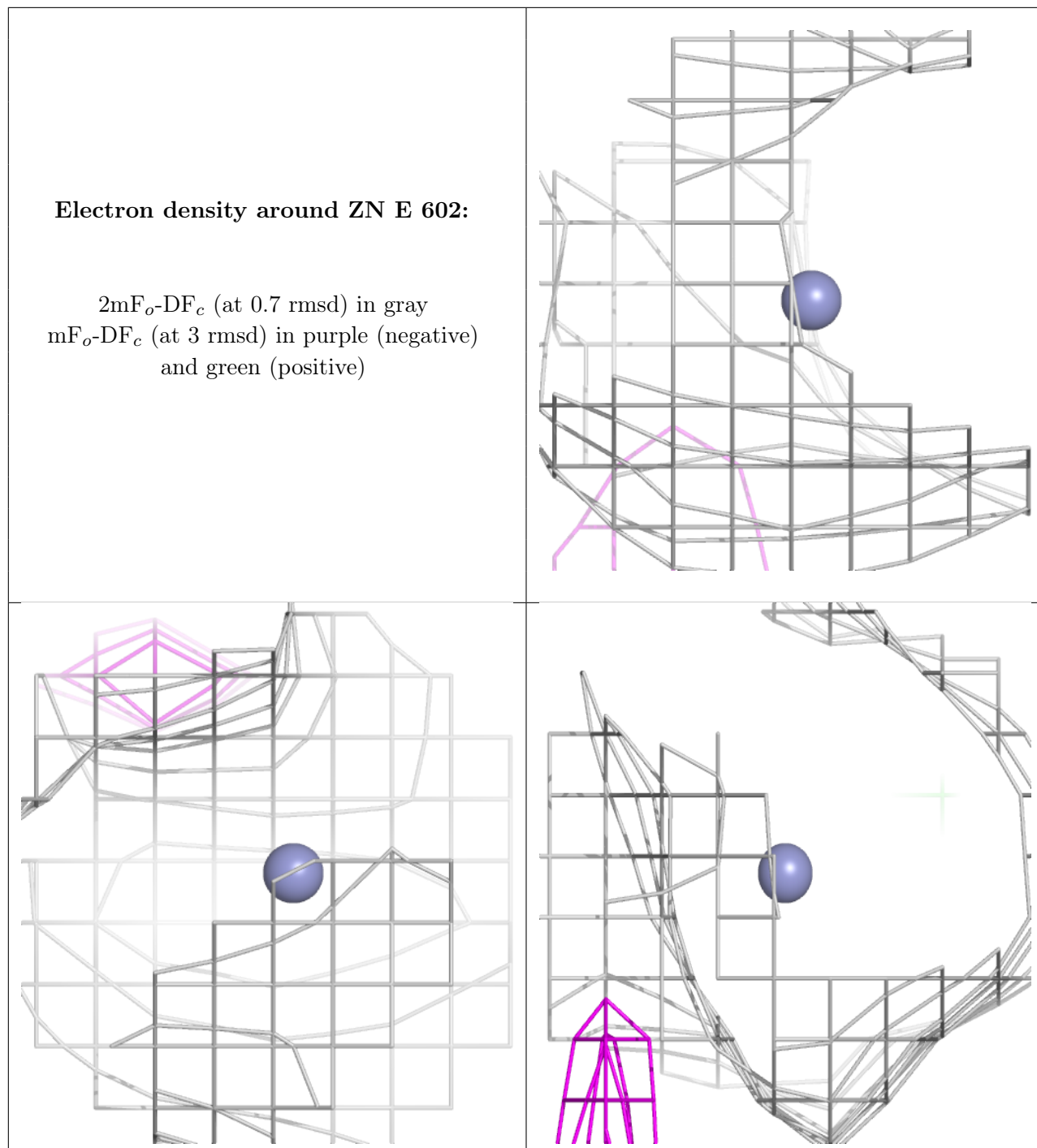
Electron density around PO4 C 606:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



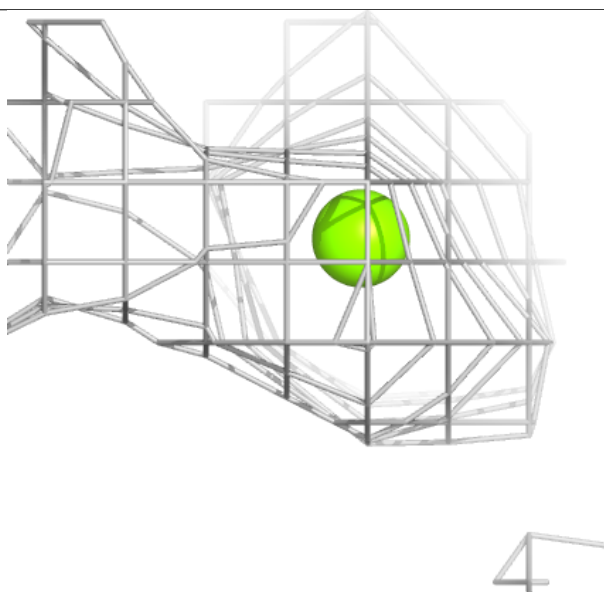
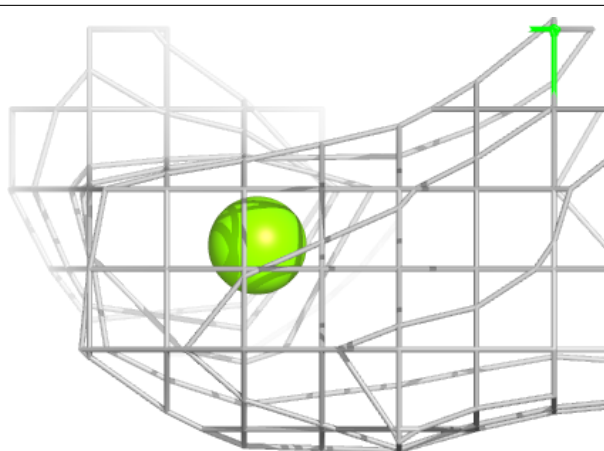
Electron density around ZN E 602:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



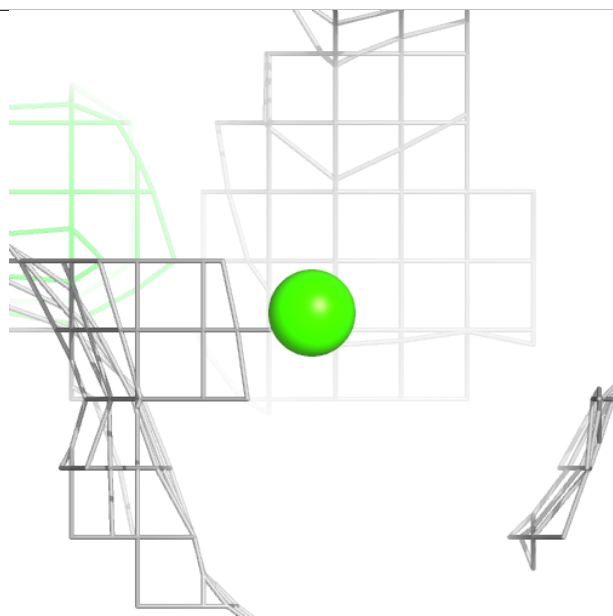
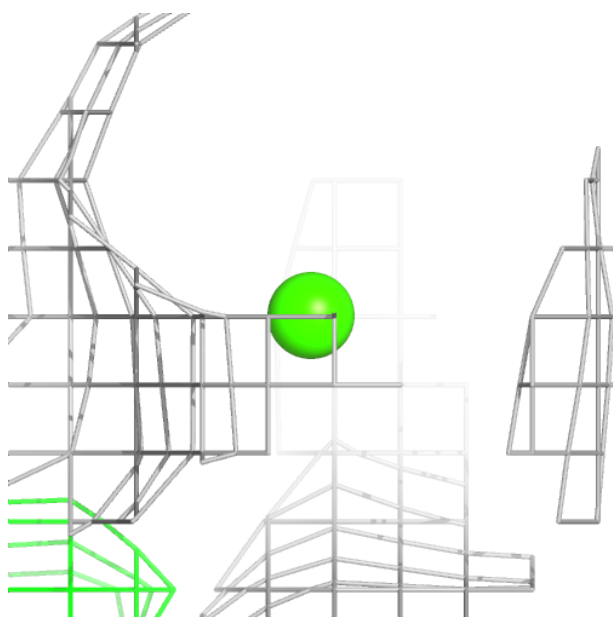
Electron density around MG B 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



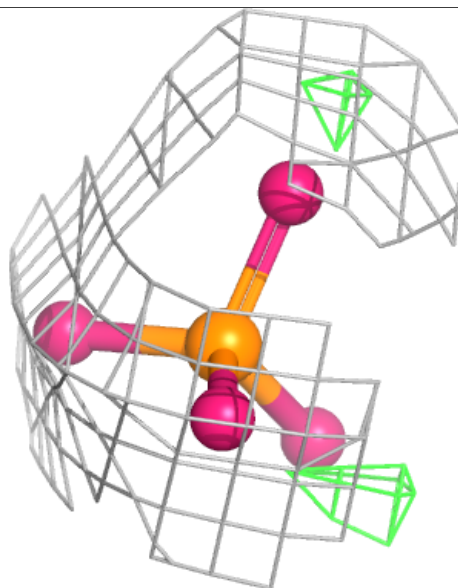
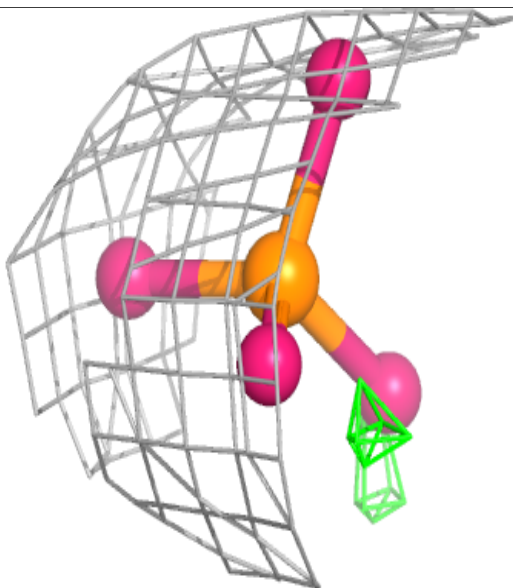
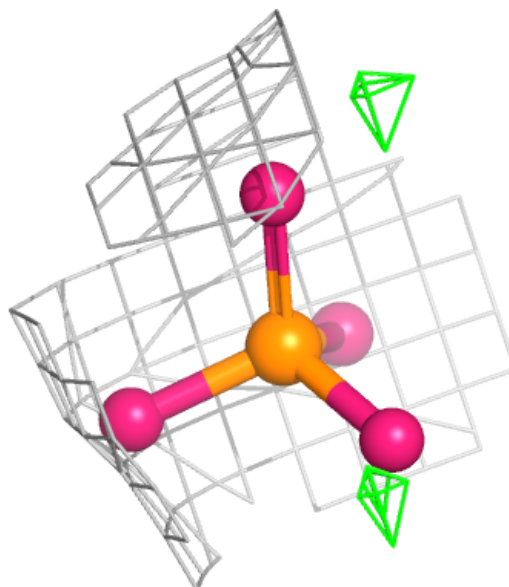
Electron density around CA E 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



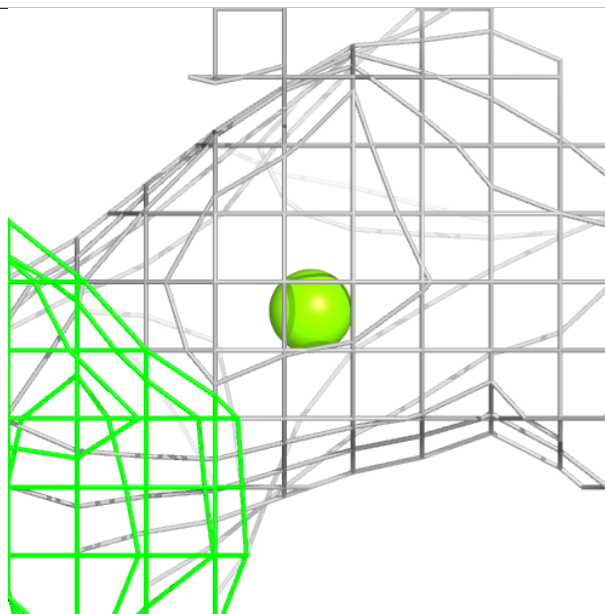
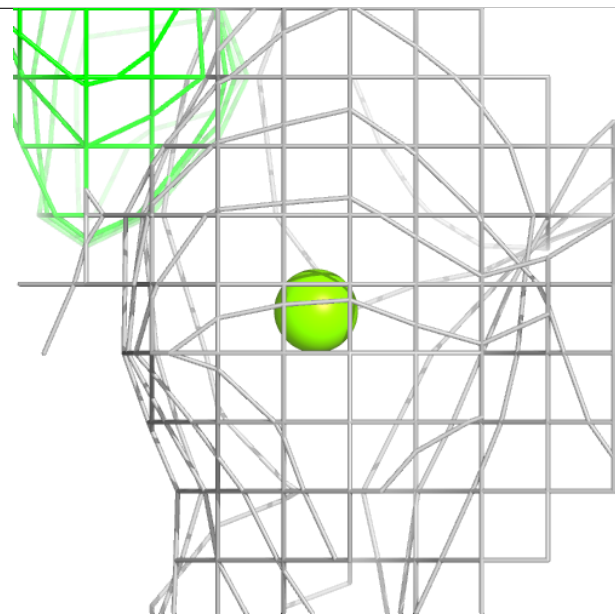
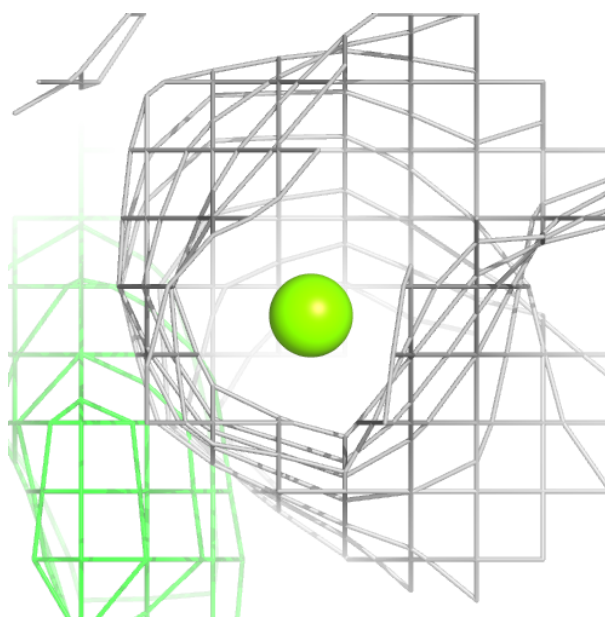
Electron density around PO4 E 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



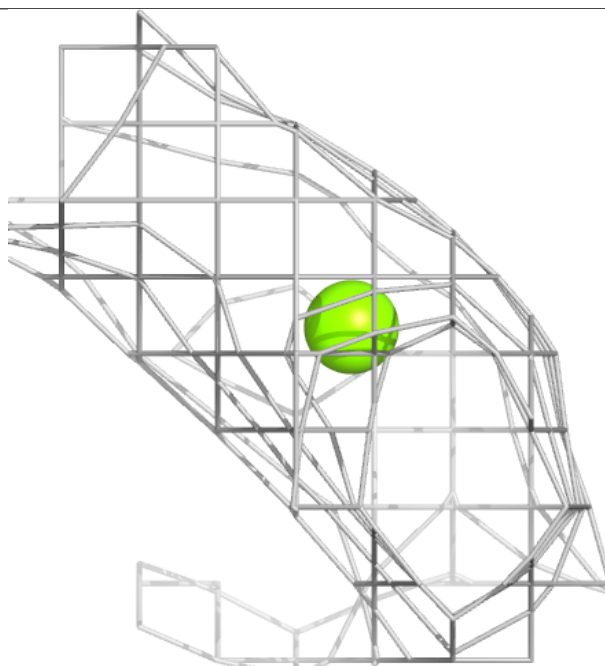
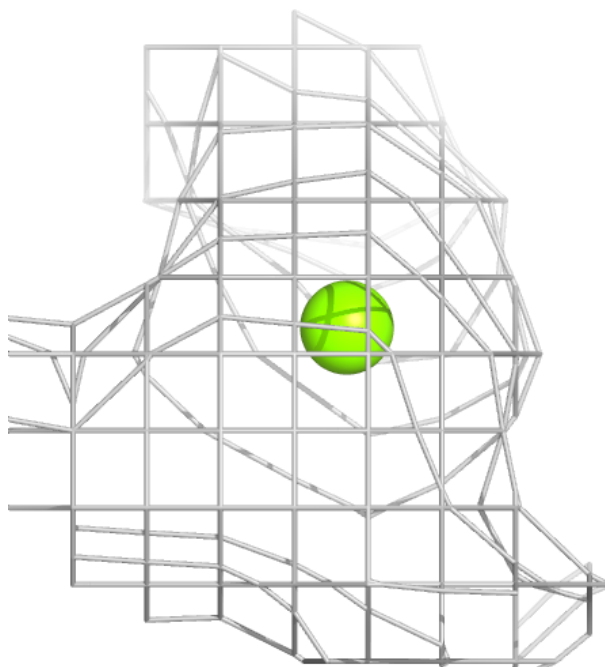
Electron density around MG A 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



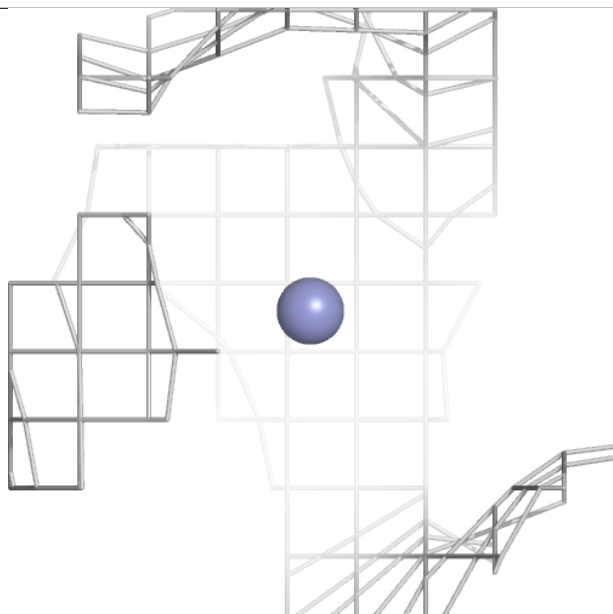
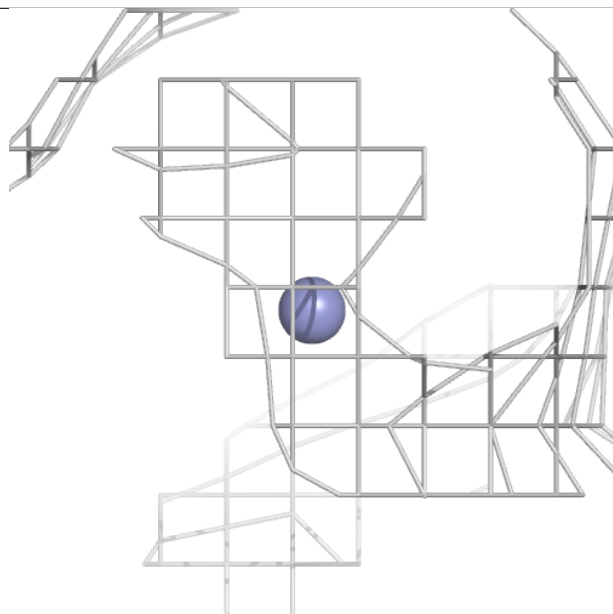
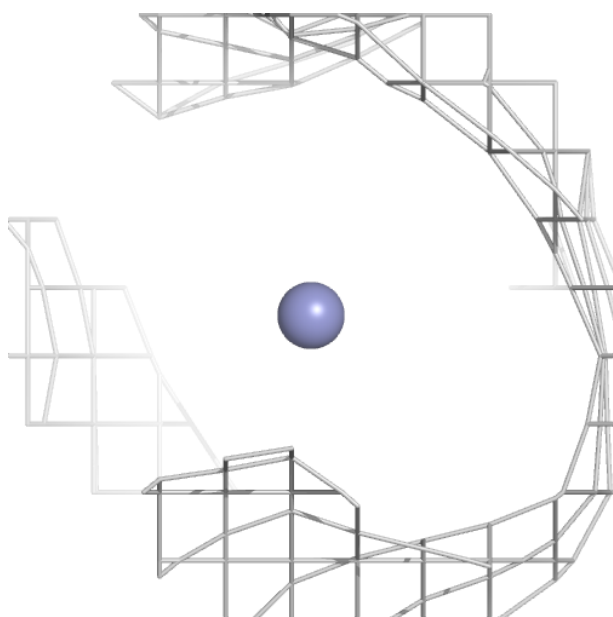
Electron density around MG D 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



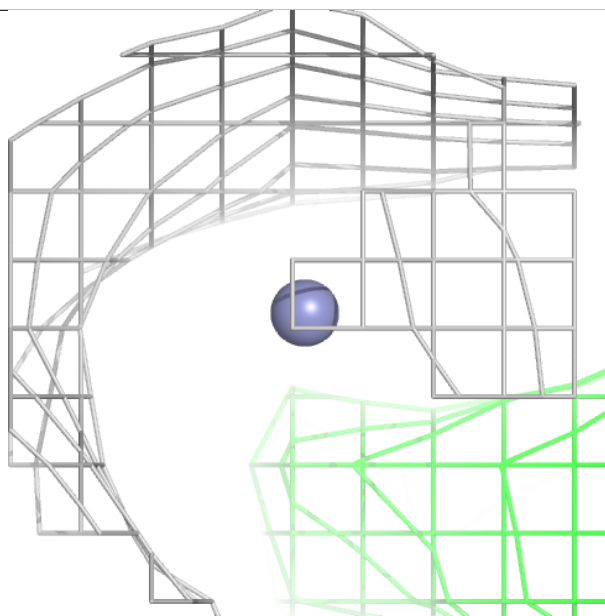
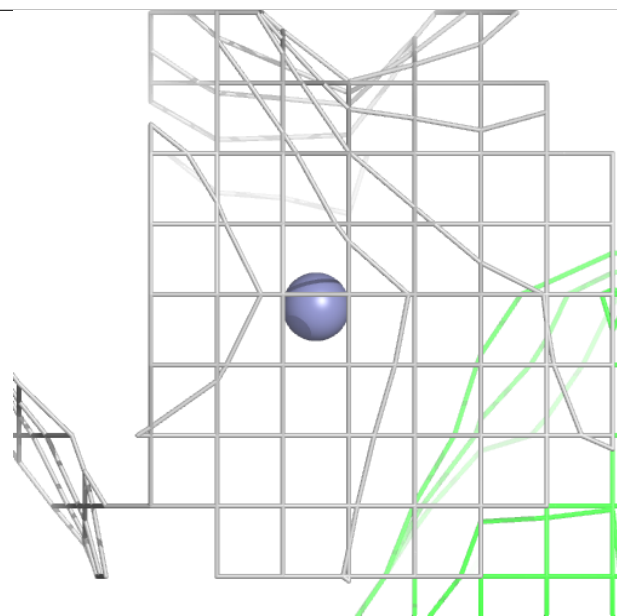
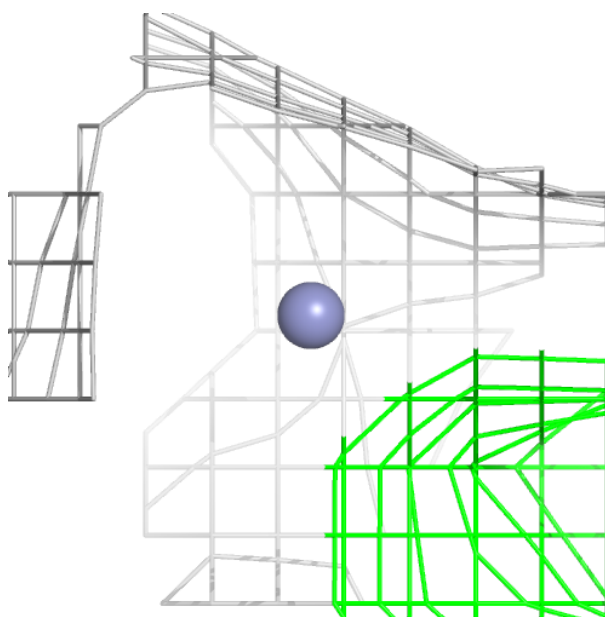
Electron density around ZN D 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



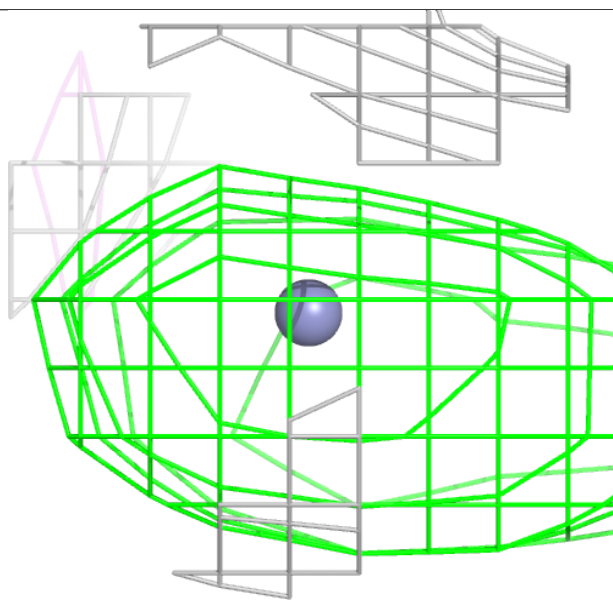
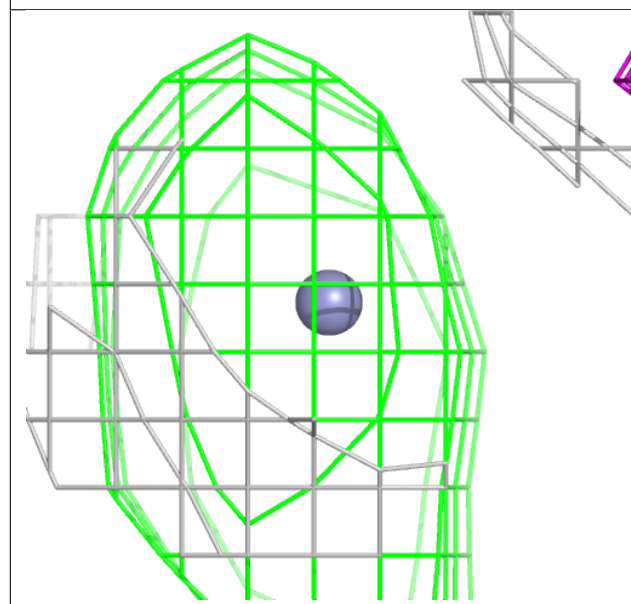
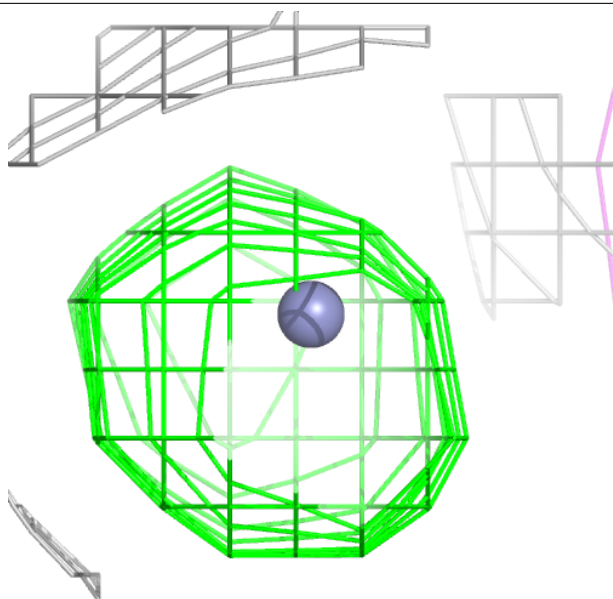
Electron density around ZN B 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



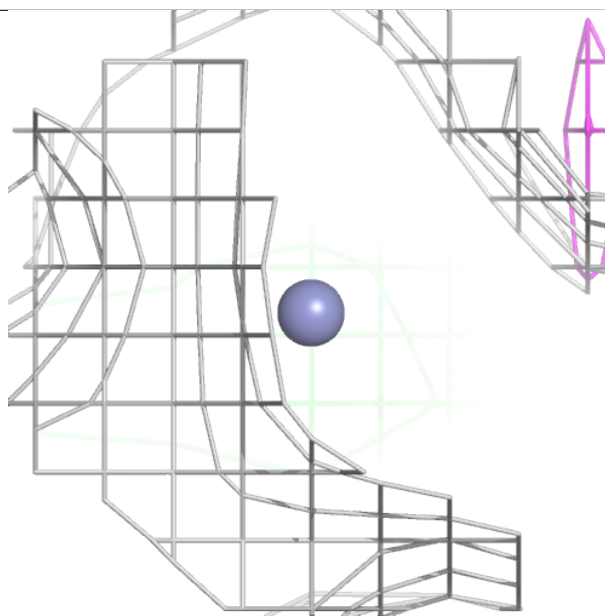
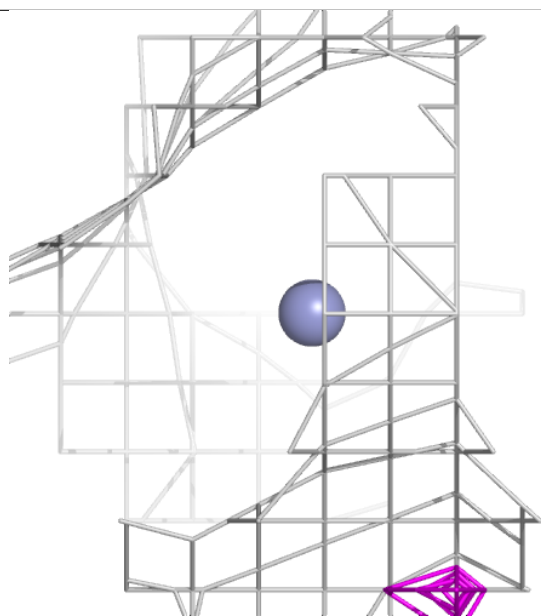
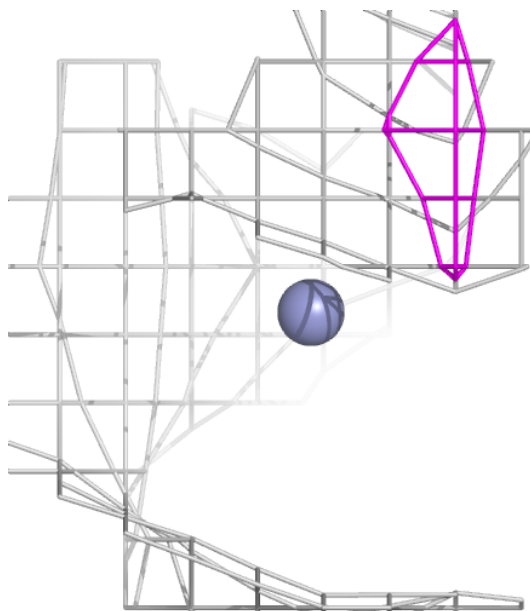
Electron density around ZN C 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



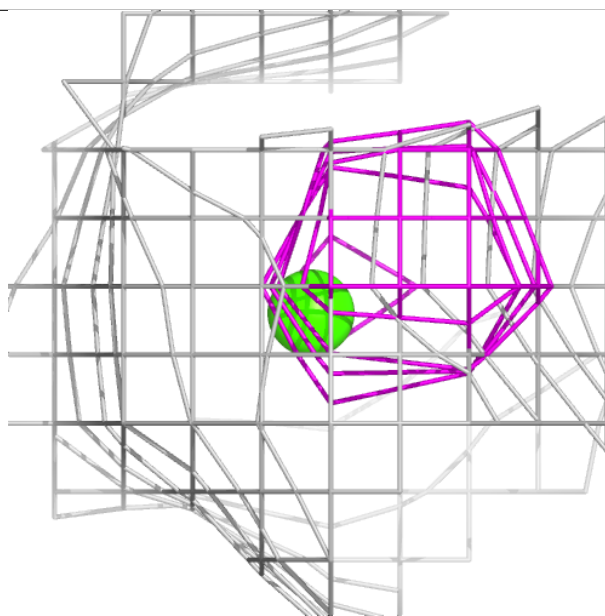
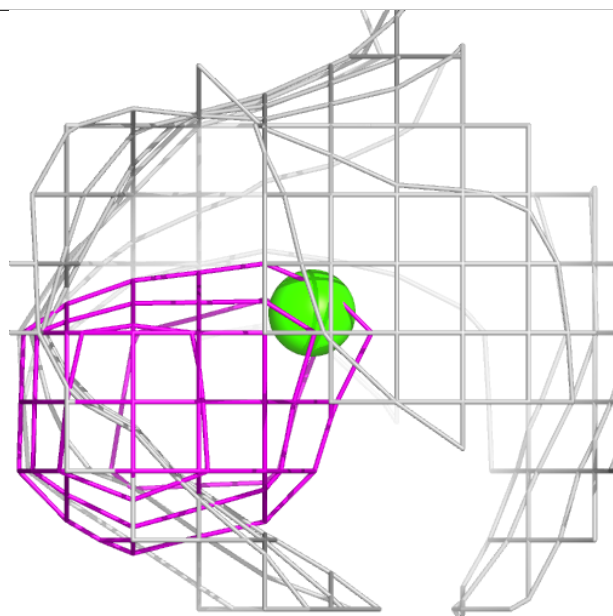
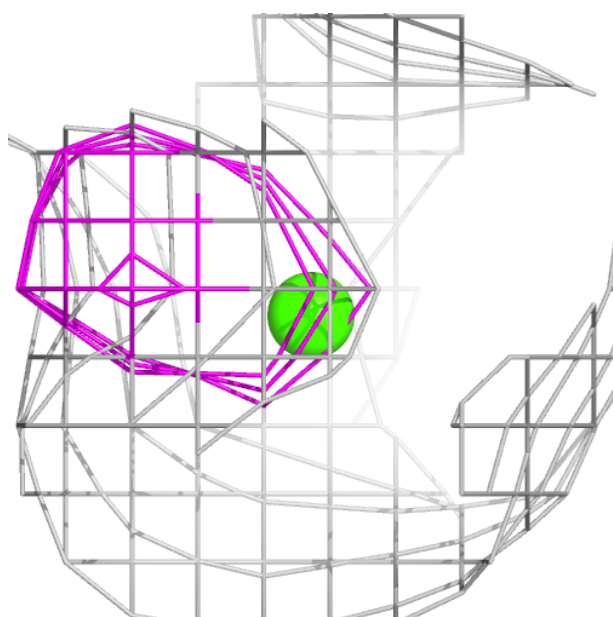
Electron density around ZN C 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



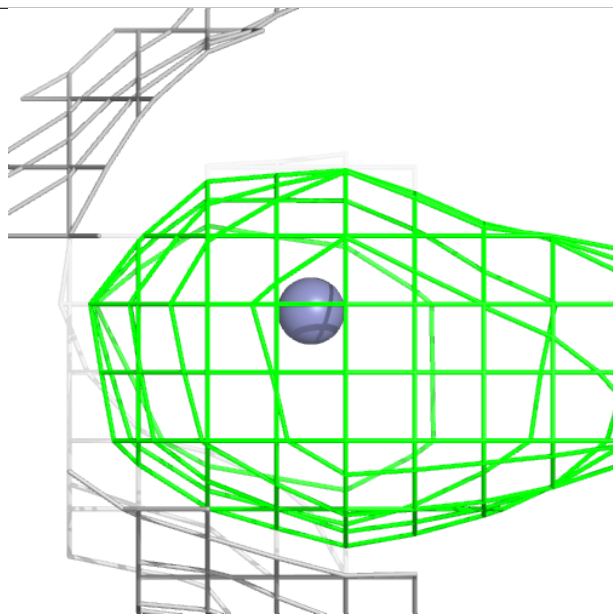
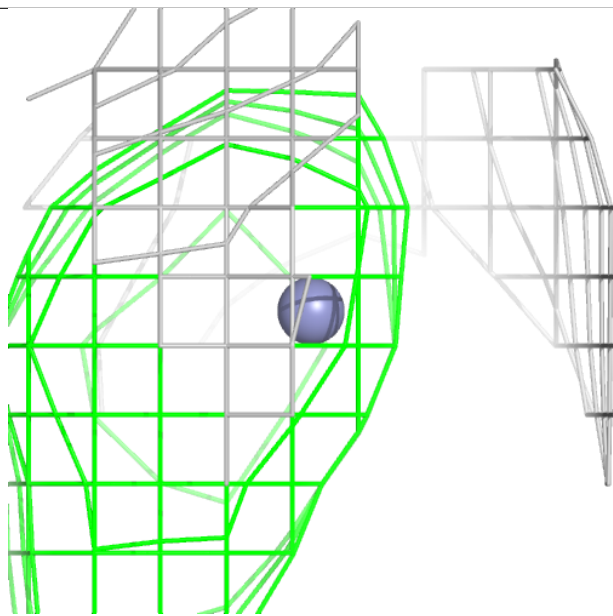
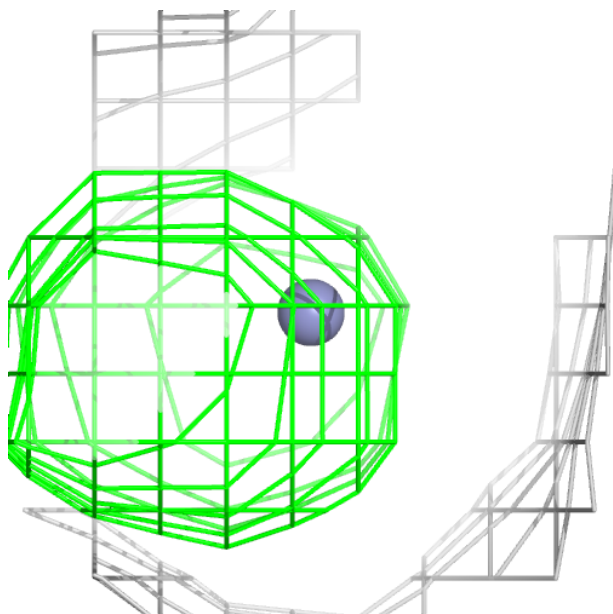
Electron density around CA A 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



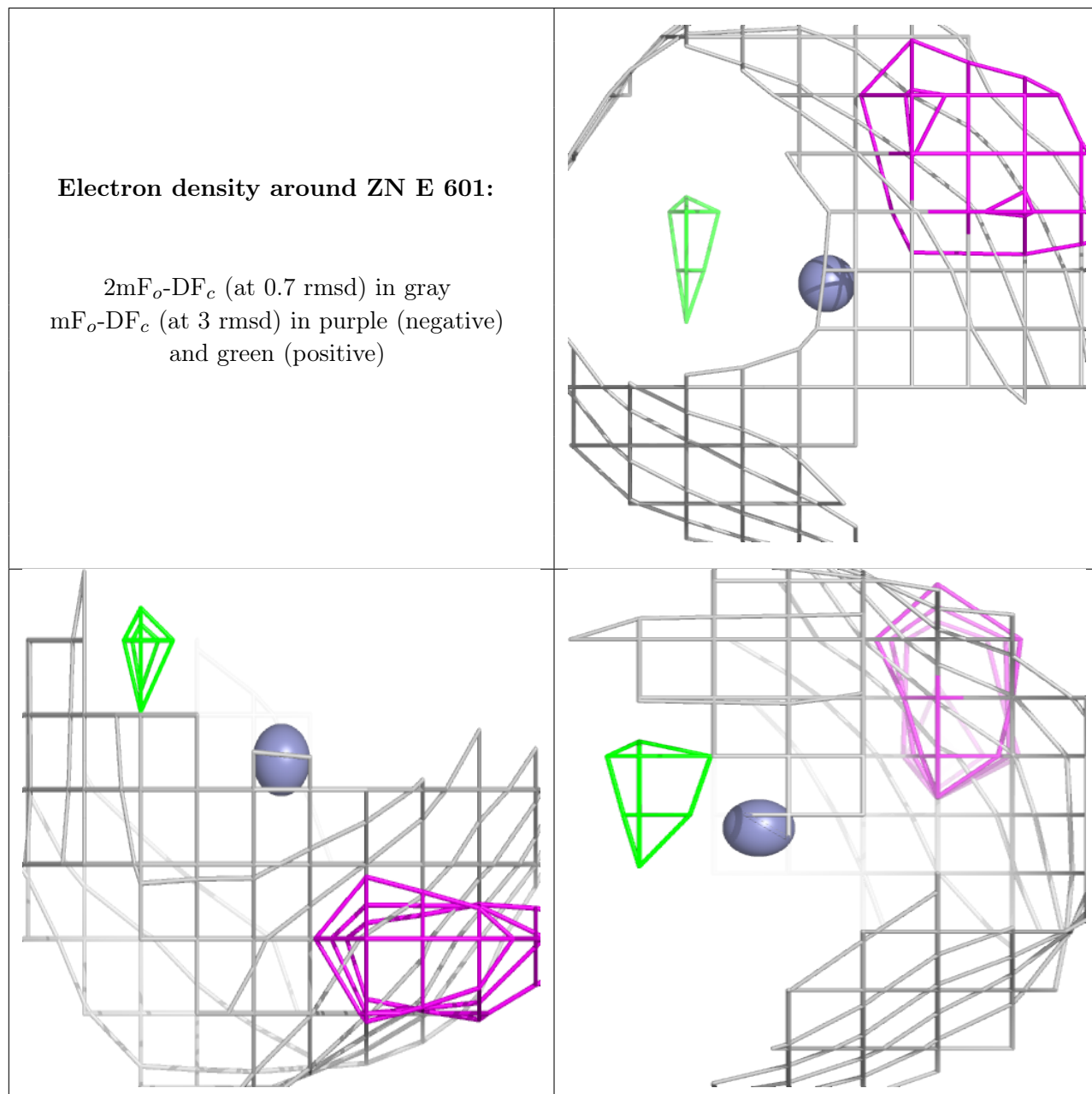
Electron density around ZN B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



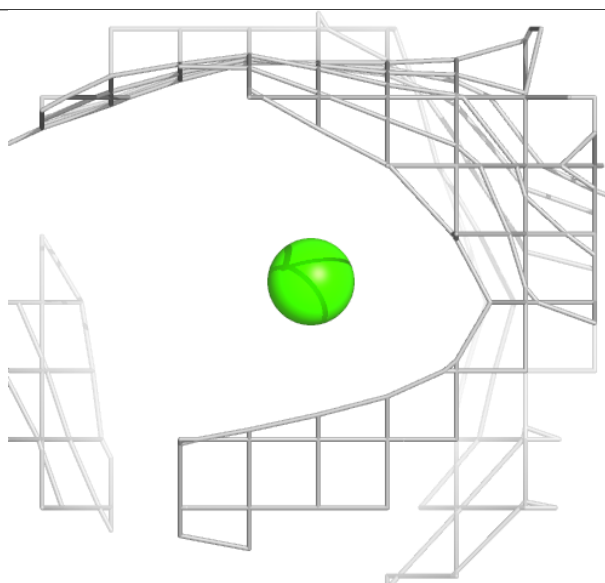
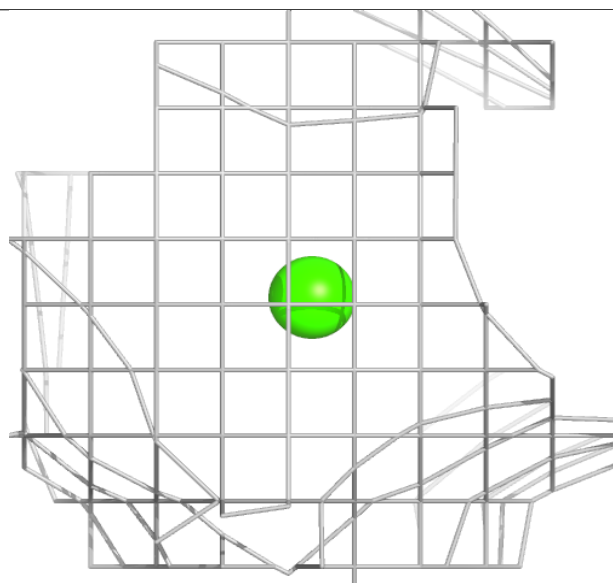
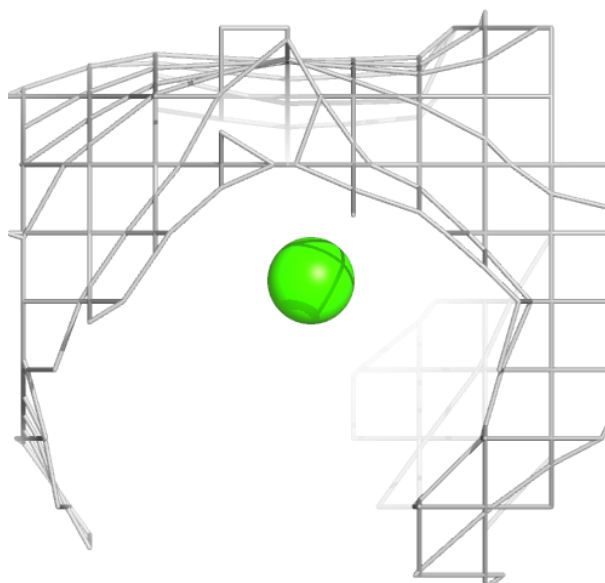
Electron density around ZN E 601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



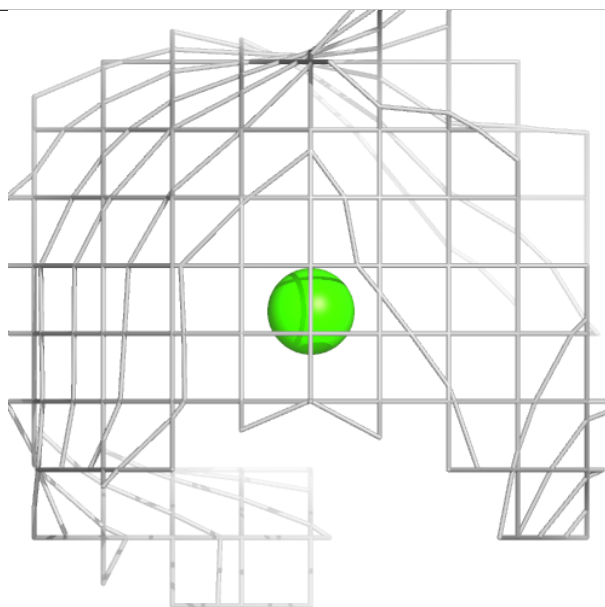
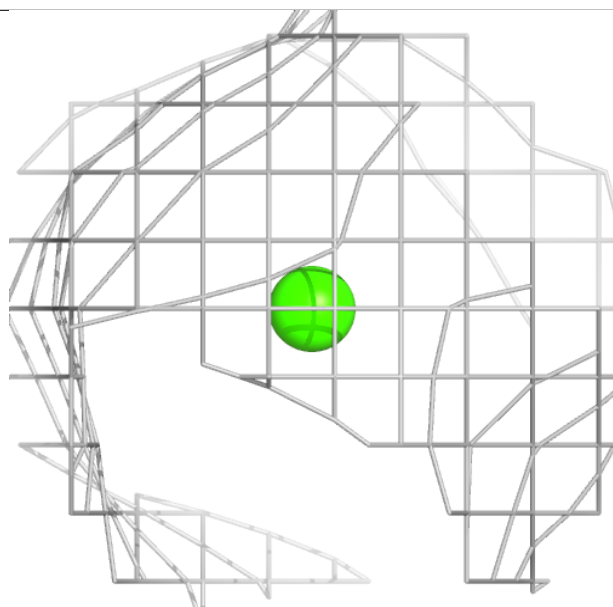
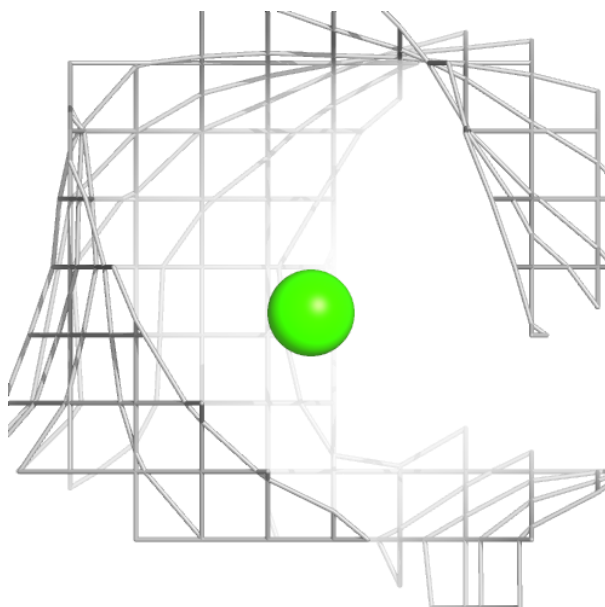
Electron density around CA B 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



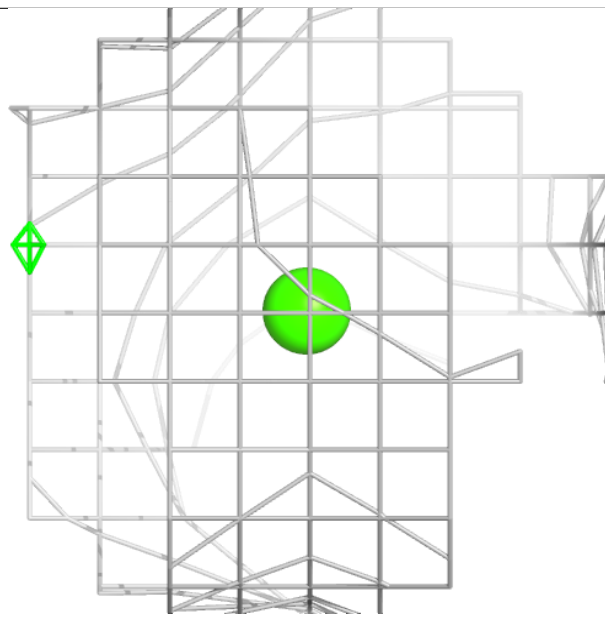
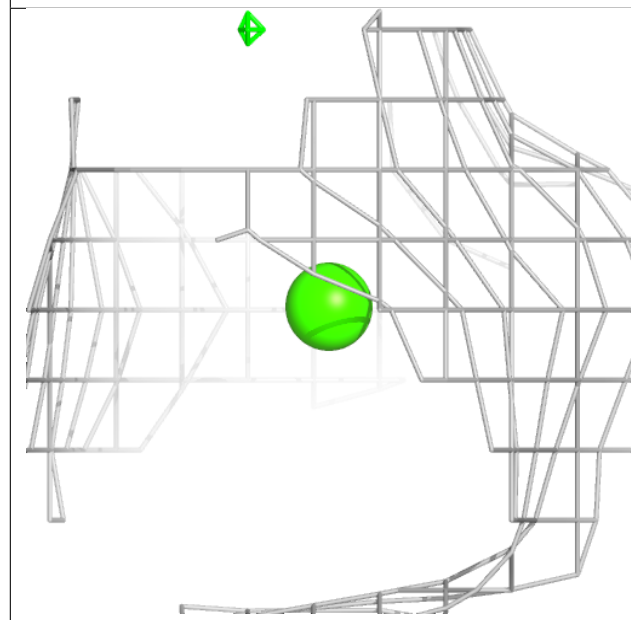
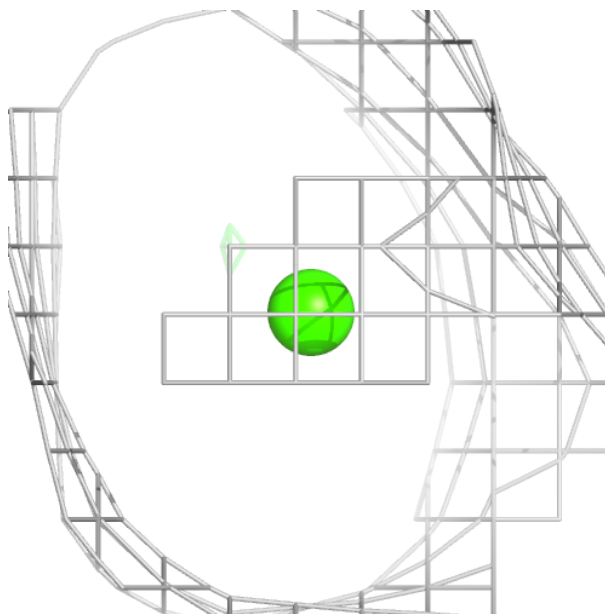
Electron density around CA C 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



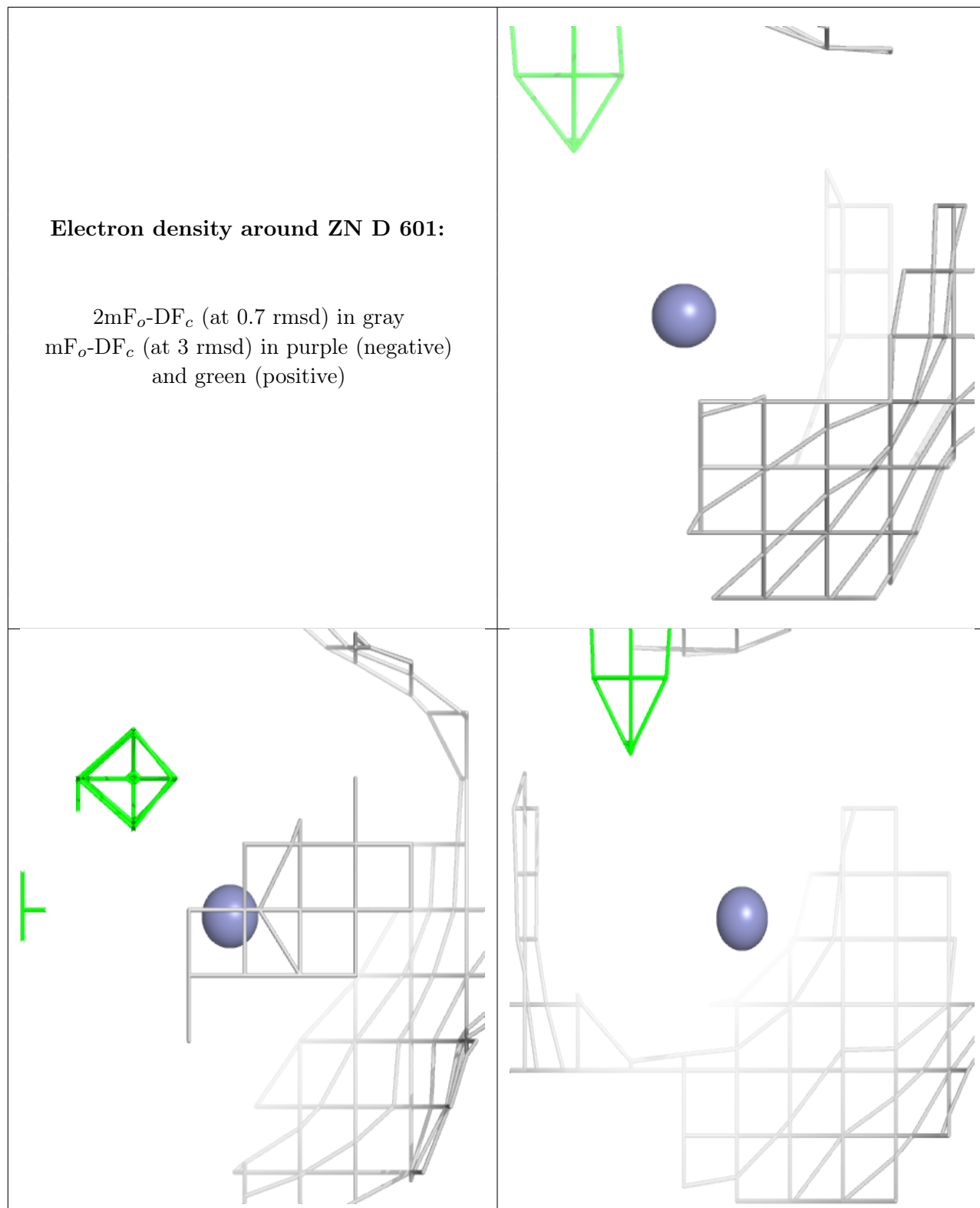
Electron density around CA D 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



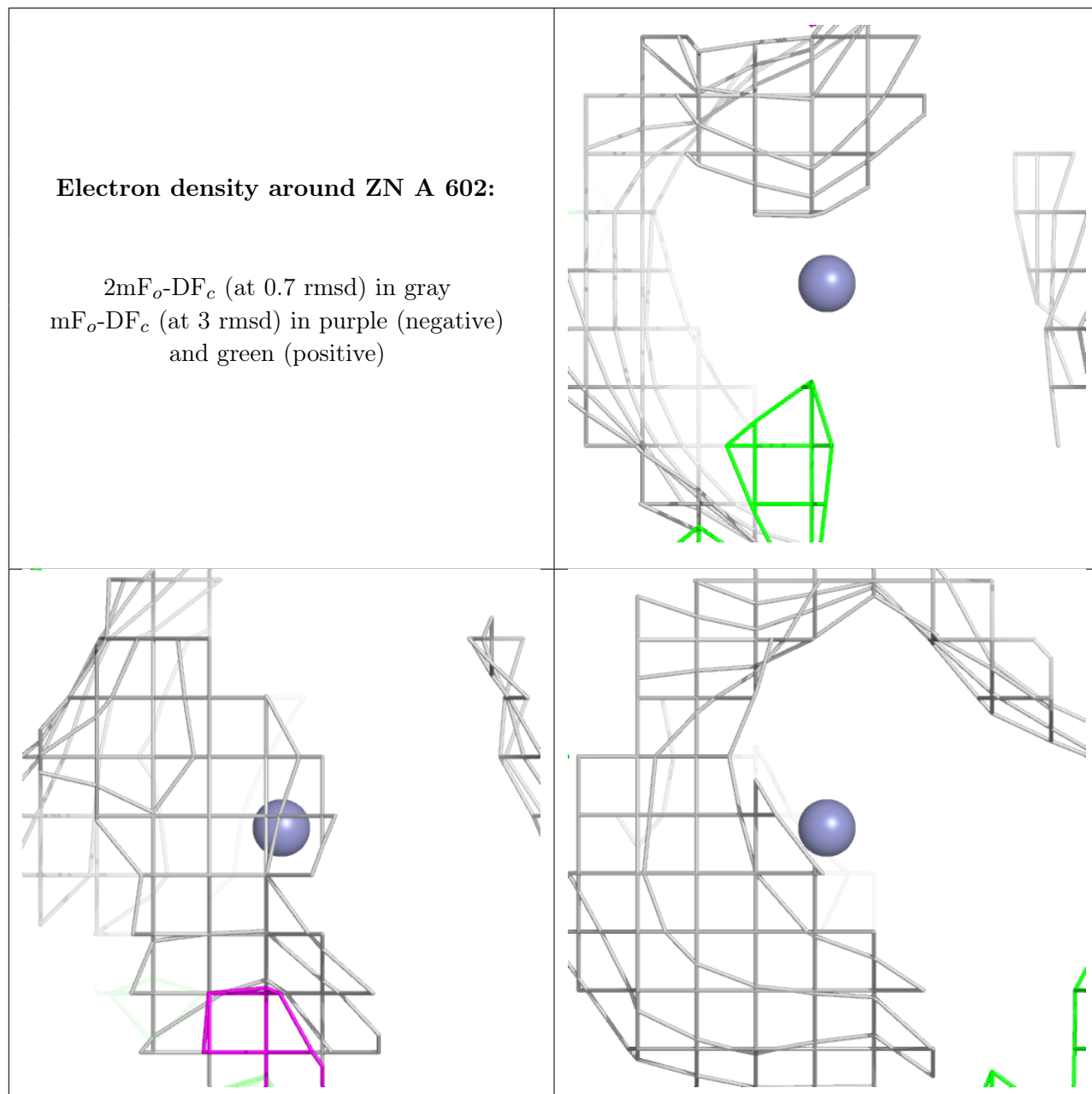
Electron density around ZN D 601:

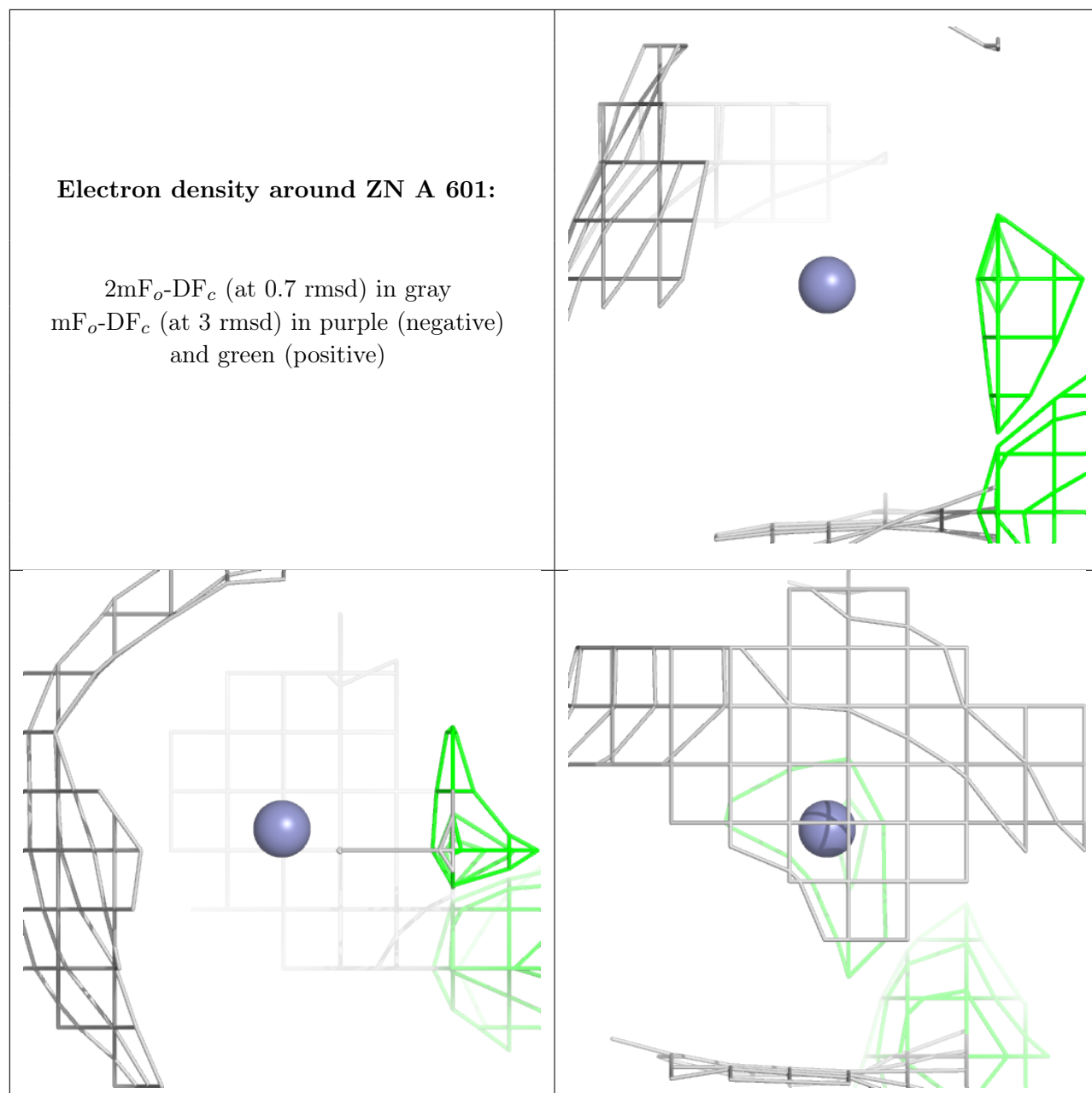
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.